

STIC-EIC1800/2900

288329

From: SEAN BASQUILL [sean.basquill@uspto.gov]
Sent: Friday, March 06, 2009 10:48 AM
To: STIC-EIC1800/2900
Subject: Search Request, Case/Application No.: 10560012

Requester: SEAN BASQUILL (P/1612)
Art Unit: GROUP ART UNIT 1612

Case/Application number: 10560012
Priority Filing Date: 10 June 2003
Format for Search Results: Email
Meaning of unusual acronyms or initialisms:

Identify the novelty:

Claim 29, as attached, recites approximately four-and-a-half pages of discrete chemical compound names of species within a genus as claimed. I would like to know if any of the compounds were known in the art prior to June 10, 2003.

Additional comments:

ONLY the chemical compounds as recited in Claim 29 (which yes, goes on for five pages) are of concern here.

Attachment: Yes (10560012 Claim 29.pdf)

M9
3/6/2009

=> file registry

FILE 'REGISTRY' ENTERED AT 11:02:00 ON 12 MAR 2009

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Property values tagged with IC are from the ZIC/VINITI data file

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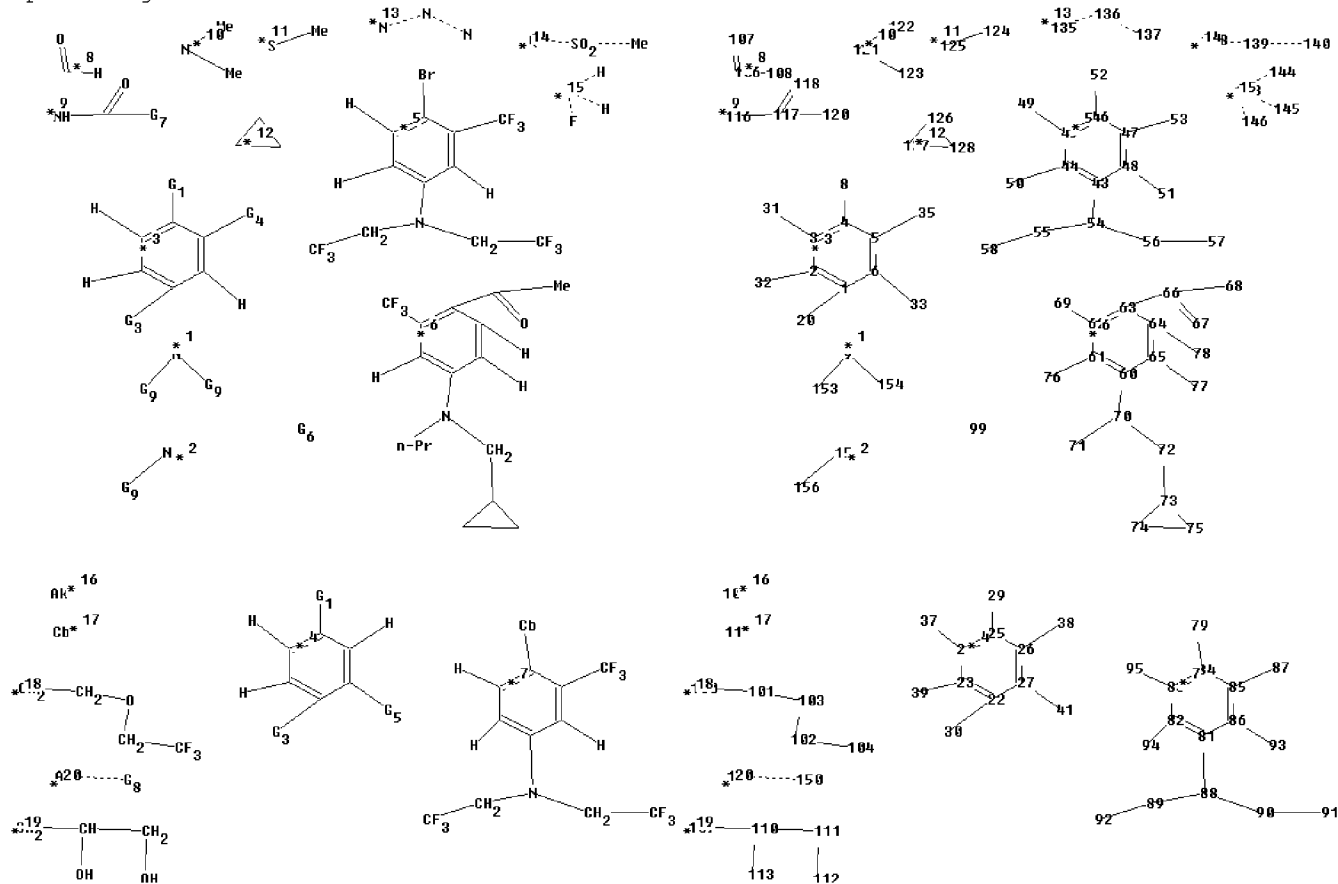
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

Uploading L26.str



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8  9  10  11  15  20  29  30  31  32  33  35  37  38  39  41  49  50  51  52  53
54  55  56  57  58  66  67  68  69  70  71  72  76  77  78  79  87  88  89  90  91
92  93  94  95
99  100  101  102  103  104  106  107  108  109  110  111  112  113  115  116  117
118  120  121
122  123  124  125  135  136  137  138  139  140  143  144  145  146  150  153  154
156
ring nodes :

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```
1  2  3  4  5  6 22 23 24 25 26 27 43 44 45 46 47 48 60 61 62 63
64 65 73 74 75 81 82 83 84 85 86 126 127 128
chain bonds :
1-20  2-32  3-31  4-8   5-35  6-33  9-153 9-154 15-156 22-30 23-39 24-37 25-29
26-38 27-41 43-54 44-50 45-49 46-52 47-53 48-51 54-55 54-56 55-58 56-57
60-70 61-76
62-69 63-66 64-78 65-77 66-67 66-68 70-71 70-72 72-73 79-84 81-88 82-94
83-95 85-87
86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108
106-107 109-110
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123
124-125 135-136
136-137 138-139 139-140 143-144 143-145 143-146
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75
74-75 81-82
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128
exact/norm bonds :
1-20  4-8  5-35  9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120
126-127 126-128
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146
exact bonds :
2-32  3-31  6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73
79-84 82-94 83-95
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-
108 109-110
110-111 111-112 121-122 121-123 124-125
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86
82-83 83-84
84-85 85-86
isolated ring systems :
containing 1 : 22 : 43 : 60 : 81 :
```

G1:CN,NO2

G3:[*1],[*2]

G4:CF3,C1,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,C1

G6:[*3],[*4],[*5],[*6],[*7]

G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15]

G9:[*16],[*17],[*18],[*19],[*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

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9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain
125:2 E exact
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS
30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom
44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS
54:CLASS 55:CLASS
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom
66:CLASS
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom
75:Atom 76:CLASS 77:CLASS
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS
88:CLASS
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS
100:CLASS 101:CLASS
102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 111:CLASS
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS
121:CLASS 122:CLASS
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS
137:CLASS
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS
150:CLASS 153:CLASS
154:CLASS 156:CLASS

Generic attributes :

11:
Saturation : Saturated
79:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

Element Count :

Node 10: Limited
C,C7

Node 11: Limited
C,C6

Node 79: Limited
C,C6

Node 115: Limited
C,C6

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 11:02:04 ON 12 MAR 2009

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10/560012

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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L69

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      82177
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10/560012

L14 SCR 616
L26 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L27 SCR 1993
L32 SCR 1840 OR 2043 OR 1951
L35 898352 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (N>1 AND ((46.150.18/
RID AND 1/NRS) OR (46.150.18/RID AND (1.13.1/RID OR 16.127.1/RI
D OR 46.150.1/RID) AND 2/NRS))) NOT PMS/CI
L38 1054 SEA FILE=REGISTRY SUB=L35 SSS FUL L26 AND ((L14 AND L27) NOT
L32)
L47 135 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L38 AND L3
L48 16 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L3 NOT L47
L50 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 AND BR/ELS AND
9/F
L51 10 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L48 NOT BR/ELS
L52 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L51 AND F/ELS
L53 7 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L50 OR L52
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L56 359 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L55 AND L38
L66 142 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L55 AND L54
L67 366 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L56 OR L66
L68 68 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L67
L69 1 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L68 AND L1

10/560012

=> d ibib abs hitstr L69 1

L69 ANSWER 1 OF 1 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:14359 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:113710

TITLE: Preparation of substituted anilines as androgen receptor modulators

INVENTOR(S): Blanc, Jean-Baptiste E.; Cadilla, Rodolfo; Cowan, David John; Kaldor, Istvan; Larkin, Andrew L.; Stewart, Eugene Lee; Turnbull, Philip Stewart; Trump, Ryan Paul

PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

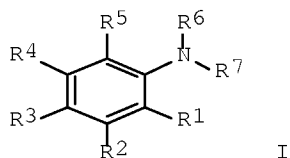
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005000795	A2	20050106	WO 2004-US18252	20040609
WO 2005000795	A3	20050310		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1654221	A2	20060510	EP 2004-776383	20040609
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR			
JP 2007500245	T	20070111	JP 2006-533629	20040609
US 20060148893	A1	20060706	US 2005-560012	20051208 <--
PRIORITY APPLN. INFO.:			US 2003-477252P	P 20030610
			WO 2004-US18252	W 20040609
OTHER SOURCE(S):	MARPAT 142:113710			
GI				



AB This invention relates to non-steroidal compds. I [R1, R2, R4, R5 = H, CN, NO2, halo, etc. (at least one of R1, R2, R4, R5 is not H); R3 = CN, NO2, halo, etc.; R6, R7 = H, (Ra)xR9 (Ra = alkylene; x = 0-1; R9 = alkyl, haloalkyl,

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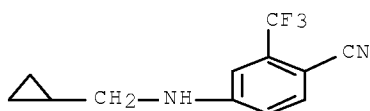
hydroxyalkyl, etc.)) that are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. Thus, reacting 4-fluoro-2-trifluoromethylbenzonitrile with N-(cyclopropylmethyl)-N-propylamine afforded 81% I [R1, R2, R5 = H; R3 = CN; R4 = CF3; R6 = CH2(cyclopropyl); R7 = Pr]. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given). The pharmaceutical composition comprising the compound I is disclosed.

IT 821777-24-6P 821777-27-9P 821777-32-6P
821777-34-8P 821777-36-0P 821777-37-1P
821777-38-2P 821777-41-7P 821777-42-8P
821777-44-0P 821777-50-8P 821777-58-6P
821777-66-6P 821777-68-8P 821777-73-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of substituted anilines as androgen receptor modulators)

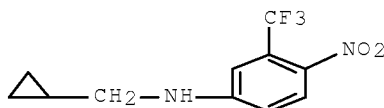
RN 821777-24-6 ZCAPLUS

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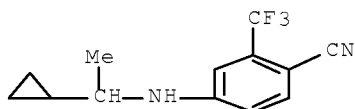
RN 821777-27-9 ZCAPLUS

CN Benzenamine, N-(cyclopropylmethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-32-6 ZCAPLUS

CN Benzonitrile, 4-[(1-cyclopropylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

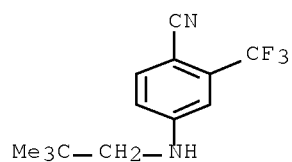


RN 821777-34-8 ZCAPLUS

CN Benzonitrile, 4-[(2,2-dimethylpropyl)amino]-2-(trifluoromethyl)- (CA

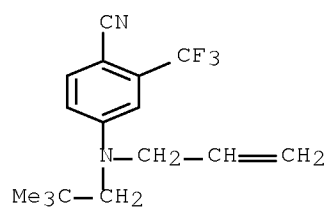
10/560012

INDEX NAME)



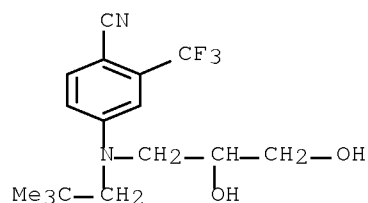
RN 821777-36-0 ZCAPLUS

CN Benzonitrile, 4-[(2,2-dimethylpropyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



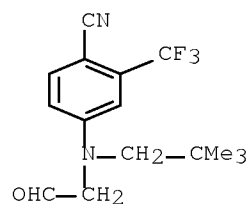
RN 821777-37-1 ZCAPLUS

CN Benzonitrile, 4-[(2,3-dihydroxypropyl)(2,2-dimethylpropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-38-2 ZCAPLUS

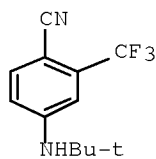
CN Benzonitrile, 4-[(2,2-dimethylpropyl)(2-oxoethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



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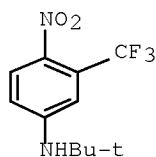
RN 821777-41-7 ZCAPLUS

CN Benzonitrile, 4-[(1,1-dimethylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



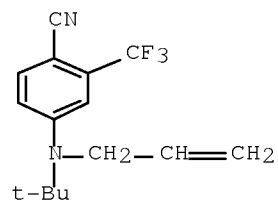
RN 821777-42-8 ZCAPLUS

CN Benzenamine, N-(1,1-dimethylethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



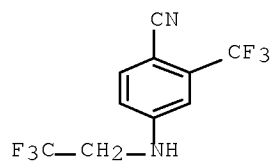
RN 821777-44-0 ZCAPLUS

CN Benzonitrile, 4-[(1,1-dimethylethyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-50-8 ZCAPLUS

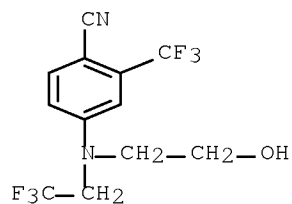
CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/560012

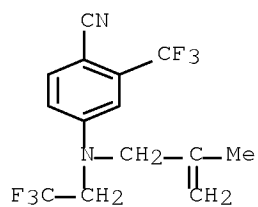
RN 821777-58-6 ZCAPLUS

CN Benzonitrile, 4-[(2-hydroxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



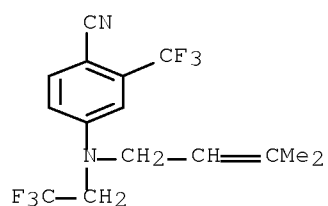
RN 821777-66-6 ZCAPLUS

CN Benzonitrile, 4-[(2-methyl-2-propen-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-68-8 ZCAPLUS

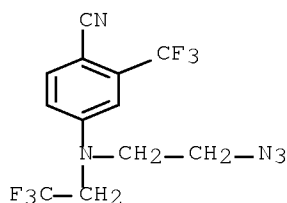
CN Benzonitrile, 4-[(3-methyl-2-buten-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-73-5 ZCAPLUS

CN Benzonitrile, 4-[(2-azidoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

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IT 51332-25-3P 115416-50-7P 151951-35-8P
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 821776-46-9P 821776-47-0P 821776-48-1P
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 821776-52-7P 821776-53-8P 821776-54-9P
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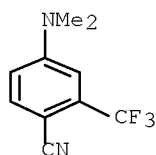
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of substituted anilines as androgen receptor modulators)

RN 51332-25-3 ZCAPLUS

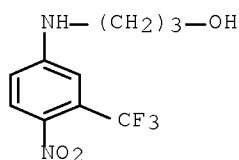
CN Benzonitrile, 4-(dimethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



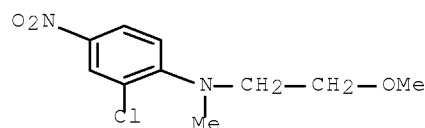
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CN 1-Propanol, 3-[[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



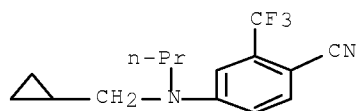
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CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



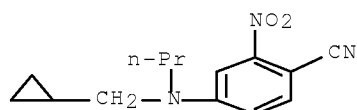
RN 821776-43-6 ZCAPLUS

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RN 821776-44-7 ZCAPLUS

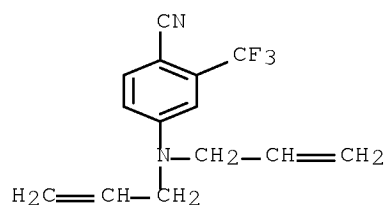
CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)



10/560012

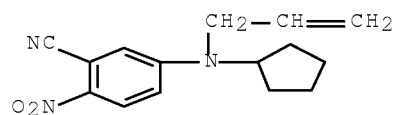
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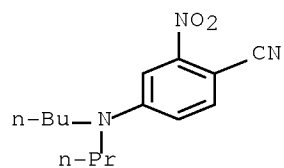
RN 821776-46-9 ZCAPLUS

CN Benzonitrile, 5-(cyclopentyl-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



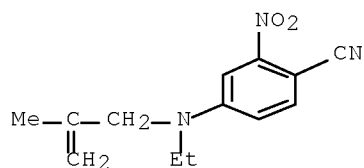
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CN Benzonitrile, 4-(butylpropylamino)-2-nitro- (CA INDEX NAME)



RN 821776-48-1 ZCAPLUS

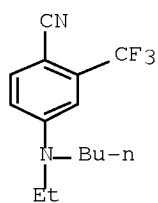
CN Benzonitrile, 4-[ethyl(2-methyl-2-propen-1-yl)amino]-2-nitro- (CA INDEX NAME)



10/560012

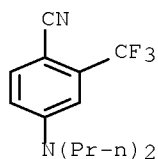
RN 821776-49-2 ZCAPLUS

CN Benzonitrile, 4-(butylethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



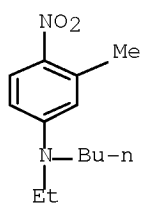
RN 821776-50-5 ZCAPLUS

CN Benzonitrile, 4-(dipropylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



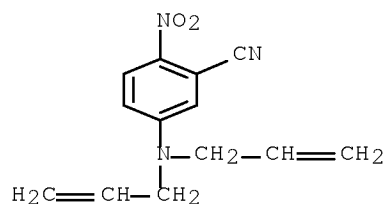
RN 821776-51-6 ZCAPLUS

CN Benzenamine, N-butyl-N-ethyl-3-methyl-4-nitro- (CA INDEX NAME)



RN 821776-52-7 ZCAPLUS

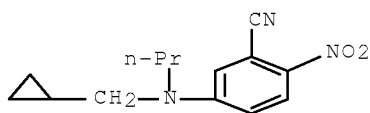
CN Benzonitrile, 5-(di-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



10/560012

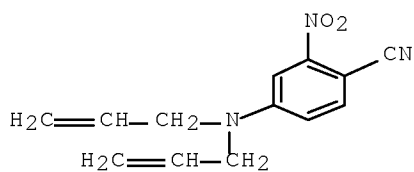
RN 821776-53-8 ZCAPLUS

CN Benzonitrile, 5-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)



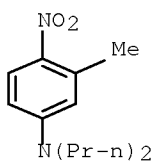
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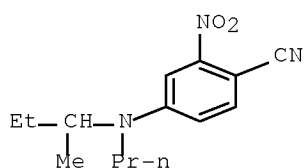
RN 821776-55-0 ZCAPLUS

CN Benzenamine, 3-methyl-4-nitro-N,N-dipropyl- (CA INDEX NAME)



RN 821776-56-1 ZCAPLUS

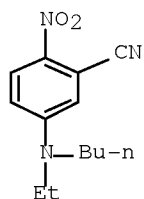
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RN 821776-57-2 ZCAPLUS

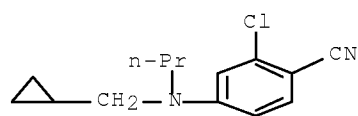
CN Benzonitrile, 5-(butylethylamino)-2-nitro- (CA INDEX NAME)

10/560012



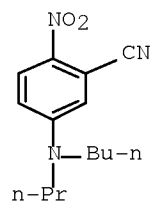
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CN Benzonitrile, 2-chloro-4-[(cyclopropylmethyl)propylamino]- (CA INDEX NAME)



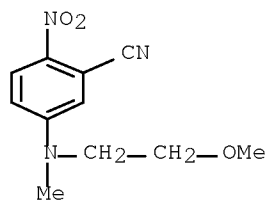
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CN Benzonitrile, 5-(butylpropylamino)-2-nitro- (CA INDEX NAME)



RN 821776-60-7 ZCAPLUS

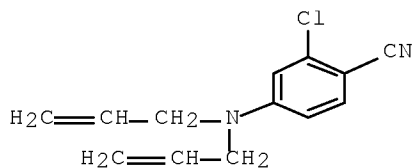
CN Benzonitrile, 5-[(2-methoxyethyl)methylamino]-2-nitro- (CA INDEX NAME)



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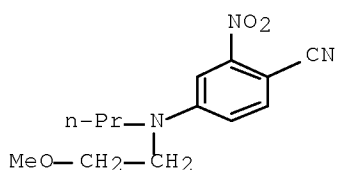
CN Benzonitrile, 2-chloro-4-(di-2-propen-1-ylamino)- (CA INDEX NAME)

10/560012



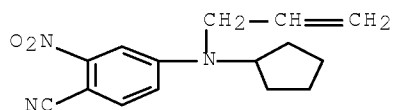
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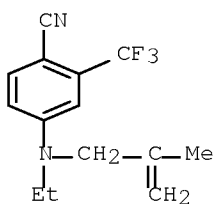
RN 821776-63-0 ZCAPLUS

CN Benzonitrile, 4-(cyclopentyl-2-propen-1-ylamino)-2-nitro- (CA INDEX NAME)



RN 821776-64-1 ZCAPLUS

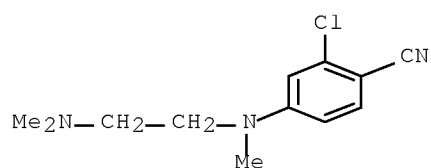
CN Benzonitrile, 4-[ethyl(2-methyl-2-propen-1-yl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821776-65-2 ZCAPLUS

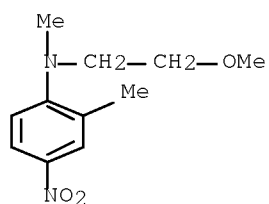
CN Benzonitrile, 2-chloro-4-[[2-(dimethylamino)ethyl]methylamino]-
(CA INDEX NAME)

10/560012



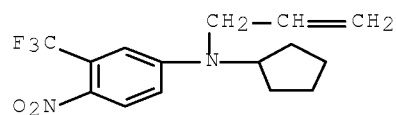
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CN Benzenamine, N-(2-methoxyethyl)-N,2-dimethyl-4-nitro- (CA INDEX NAME)



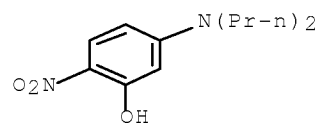
RN 821776-67-4 ZCAPLUS

CN Benzenamine, N-cyclopentyl-4-nitro-N-2-propen-1-yl-3-(trifluoromethyl)-
(CA INDEX NAME)



RN 821776-68-5 ZCAPLUS

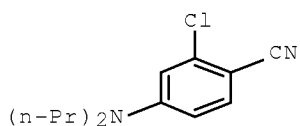
CN Phenol, 5-(dipropylamino)-2-nitro- (CA INDEX NAME)



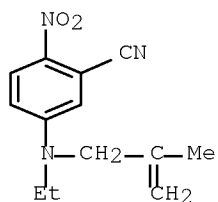
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CN Benzonitrile, 2-chloro-4-(dipropylamino)- (CA INDEX NAME)

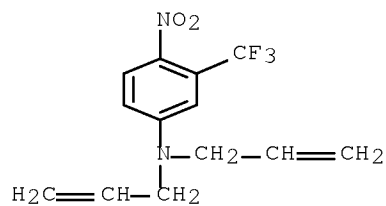
10/560012



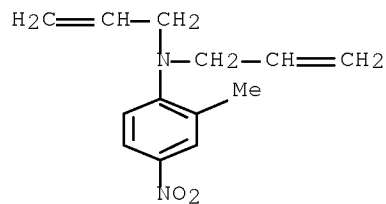
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 CN Benzonitrile, 5-[ethyl(2-methyl-2-propen-1-yl)amino]-2-nitro- (CA INDEX NAME)



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 CN Benzenamine, 4-nitro-N,N-di-2-propen-1-yl-3-(trifluoromethyl)- (CA INDEX NAME)

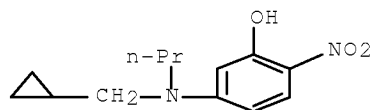


RN 821776-72-1 ZCAPLUS
 CN Benzenamine, 2-methyl-4-nitro-N,N-di-2-propen-1-yl- (CA INDEX NAME)



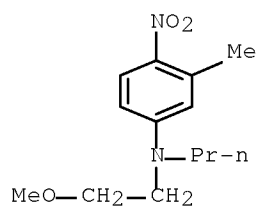
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 CN Phenol, 5-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)

10/560012



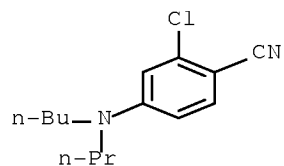
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CN Benzenamine, N-(2-methoxyethyl)-3-methyl-4-nitro-N-propyl- (CA INDEX NAME)



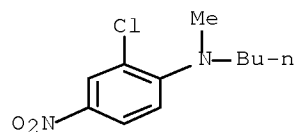
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CN Benzonitrile, 4-(butylpropylamino)-2-chloro- (CA INDEX NAME)



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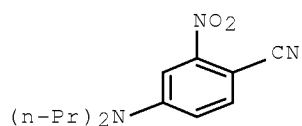
CN Benzenamine, N-butyl-2-chloro-N-methyl-4-nitro- (CA INDEX NAME)



RN 821776-77-6 ZCAPLUS

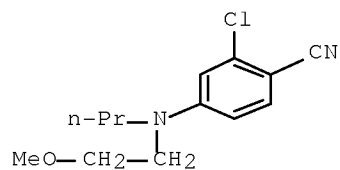
CN Benzonitrile, 4-(dipropylamino)-2-nitro- (CA INDEX NAME)

10/560012



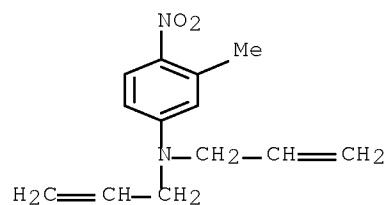
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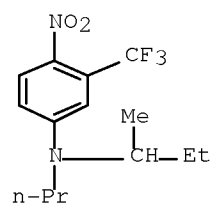
RN 821776-79-8 ZCAPLUS

CN Benzenamine, 3-methyl-4-nitro-N,N-di-2-propen-1-yl- (CA INDEX NAME)



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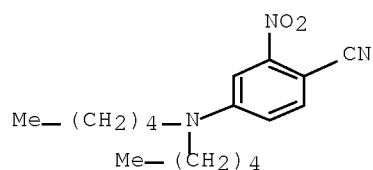
CN Benzenamine, N-(1-methylpropyl)-4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-81-2 ZCAPLUS

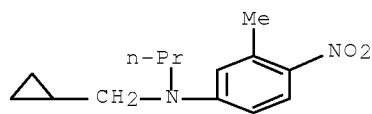
CN Benzonitrile, 4-(dipentylamino)-2-nitro- (CA INDEX NAME)

10/560012



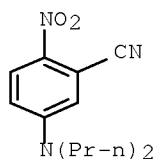
RN 821776-82-3 ZCAPLUS

CN Benzenamine, N-(cyclopropylmethyl)-3-methyl-4-nitro-N-propyl- (CA INDEX NAME)



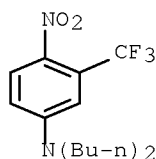
RN 821776-83-4 ZCAPLUS

CN Benzonitrile, 5-(dipropylamino)-2-nitro- (CA INDEX NAME)



RN 821776-84-5 ZCAPLUS

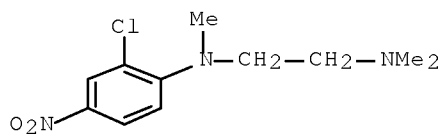
CN Benzenamine, N,N-dibutyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-85-6 ZCAPLUS

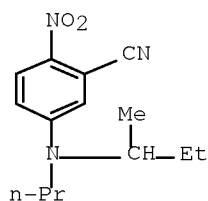
CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)

10/560012



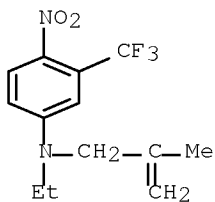
RN 821776-86-7 ZCAPLUS

CN Benzonitrile, 5-[(1-methylpropyl)propylamino]-2-nitro- (CA INDEX NAME)



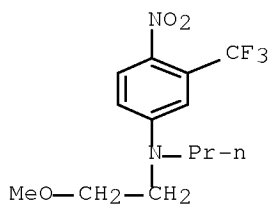
RN 821776-87-8 ZCAPLUS

CN Benzenamine, N-ethyl-N-(2-methyl-2-propen-1-yl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-88-9 ZCAPLUS

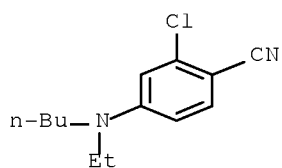
CN Benzenamine, N-(2-methoxyethyl)-4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-89-0 ZCAPLUS

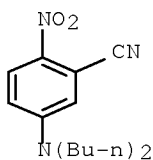
CN Benzonitrile, 4-(butylethylamino)-2-chloro- (CA INDEX NAME)

10/560012



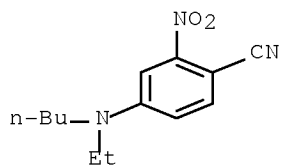
RN 821776-90-3 ZCAPLUS

CN Benzonitrile, 5-(diethylamino)-2-nitro- (CA INDEX NAME)



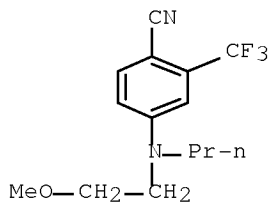
RN 821776-91-4 ZCAPLUS

CN Benzonitrile, 4-(diethylamino)-2-nitro- (CA INDEX NAME)



RN 821776-92-5 ZCAPLUS

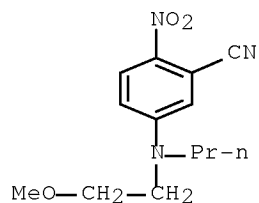
CN Benzonitrile, 4-[(2-methoxyethyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-93-6 ZCAPLUS

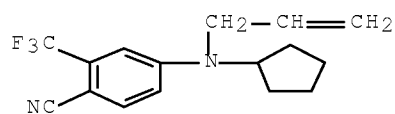
CN Benzonitrile, 5-[(2-methoxyethyl)propylamino]-2-nitro- (CA INDEX NAME)

10/560012



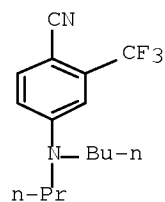
RN 821776-94-7 ZCAPLUS

CN Benzonitrile, 4-(cyclopentyl-2-propen-1-ylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



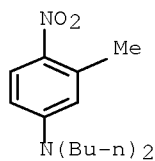
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CN Benzonitrile, 4-(butylpropylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821776-96-9 ZCAPLUS

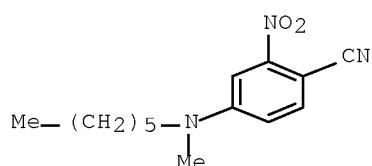
CN Benzenamine, N,N-dibutyl-3-methyl-4-nitro- (CA INDEX NAME)



RN 821776-97-0 ZCAPLUS

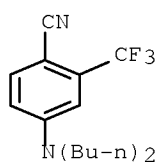
CN Benzonitrile, 4-(hexylmethylamino)-2-nitro- (CA INDEX NAME)

10/560012



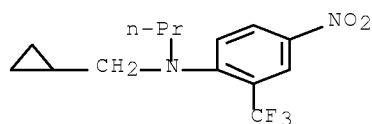
RN 821776-98-1 ZCAPLUS

CN Benzonitrile, 4-(dibutylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



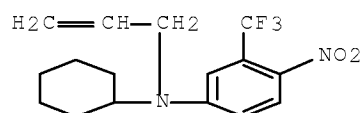
RN 821776-99-2 ZCAPLUS

CN Benzenamine, N-(cyclopropylmethyl)-4-nitro-N-propyl-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-00-8 ZCAPLUS

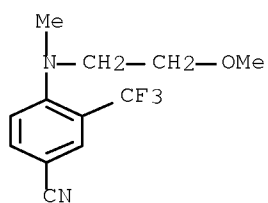
CN Benzenamine, N-cyclohexyl-4-nitro-N-2-propen-1-yl-3-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-01-9 ZCAPLUS

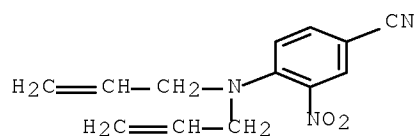
CN Benzonitrile, 4-[(2-methoxyethyl)methylamino]-3-(trifluoromethyl)-
(CA INDEX NAME)

10/560012



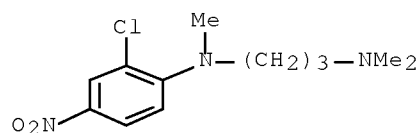
RN 821777-02-0 ZCAPLUS

CN Benzonitrile, 4-(di-2-propen-1-ylamino)-3-nitro- (CA INDEX NAME)



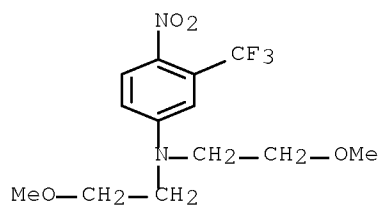
RN 821777-03-1 ZCAPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 821777-04-2 ZCAPLUS

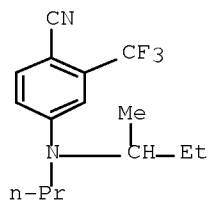
CN Benzenamine, N,N-bis(2-methoxyethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-05-3 ZCAPLUS

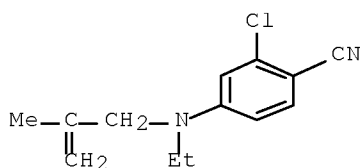
CN Benzonitrile, 4-[(1-methylpropyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



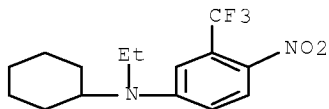
RN 821777-06-4 ZCAPLUS

CN Benzonitrile, 2-chloro-4-[ethyl(2-methyl-2-propen-1-yl)amino]- (CA INDEX NAME)



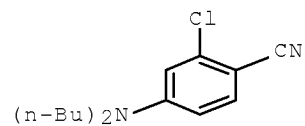
RN 821777-07-5 ZCAPLUS

CN Benzenamine, N-cyclohexyl-N-ethyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-08-6 ZCAPLUS

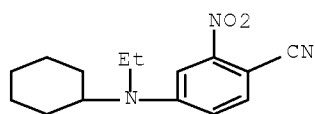
CN Benzonitrile, 2-chloro-4-(dibutylamino)- (CA INDEX NAME)



RN 821777-09-7 ZCAPLUS

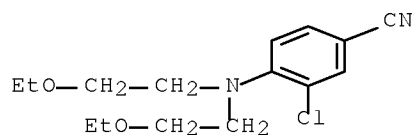
CN Benzonitrile, 4-(cyclohexylethylamino)-2-nitro- (CA INDEX NAME)

10/560012



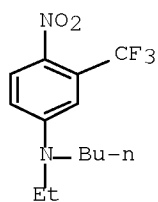
RN 821777-10-0 ZCAPLUS

CN Benzonitrile, 4-[bis(2-ethoxyethyl)amino]-3-chloro- (CA INDEX NAME)



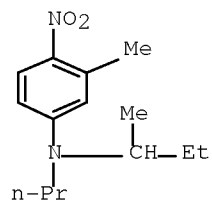
RN 821777-11-1 ZCAPLUS

CN Benzenamine, N-butyl-N-ethyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-12-2 ZCAPLUS

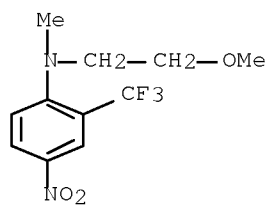
CN Benzenamine, 3-methyl-N-(1-methylpropyl)-4-nitro-N-propyl- (CA INDEX NAME)



RN 821777-13-3 ZCAPLUS

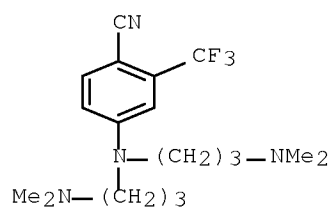
CN Benzenamine, N-(2-methoxyethyl)-N-methyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



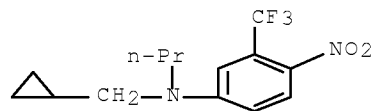
RN 821777-15-5 ZCAPLUS

CN Benzonitrile, 4-[bis[3-(dimethylamino)propyl]amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



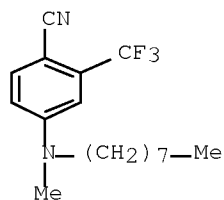
RN 821777-16-6 ZCAPLUS

CN Benzenamine, N-(cyclopropylmethyl)-4-nitro-N-propyl-3-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-17-7 ZCAPLUS

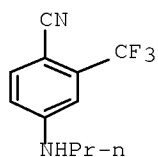
CN Benzonitrile, 4-(methyloctylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-18-8 ZCAPLUS

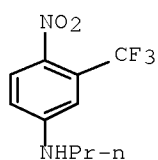
CN Benzonitrile, 4-(propylamino)-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



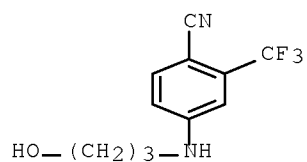
RN 821777-19-9 ZCAPLUS

CN Benzenamine, 4-nitro-N-propyl-3-(trifluoromethyl)- (CA INDEX NAME)



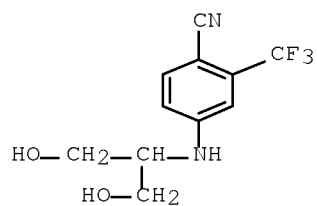
RN 821777-20-2 ZCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-21-3 ZCAPLUS

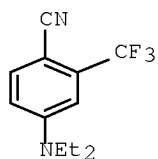
CN Benzonitrile, 4-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)



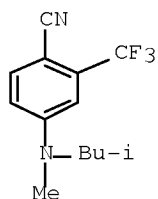
RN 821777-22-4 ZCAPLUS

CN Benzonitrile, 4-(diethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)

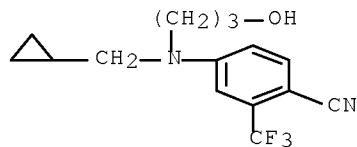
10/560012



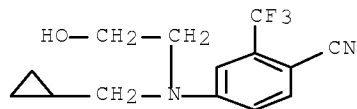
RN 821777-23-5 ZCAPLUS
CN Benzonitrile, 4-[methyl(2-methylpropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-25-7 ZCAPLUS
CN Benzonitrile, 4-[(cyclopropylmethyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

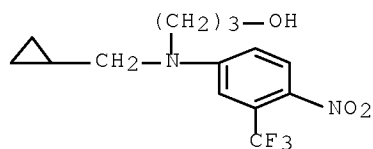


RN 821777-26-8 ZCAPLUS
CN Benzonitrile, 4-[(cyclopropylmethyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



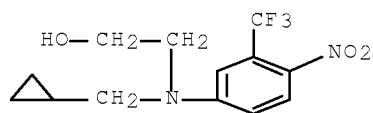
RN 821777-28-0 ZCAPLUS
CN 1-Propanol, 3-[(cyclopropylmethyl)[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

10/560012



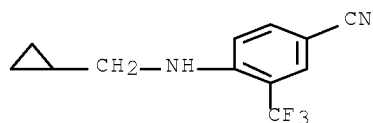
RN 821777-29-1 ZCAPLUS

CN Ethanol, 2-[(cyclopropylmethyl)[4-nitro-3-(trifluoromethyl)phenyl]amino]-
(CA INDEX NAME)



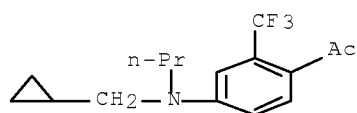
RN 821777-30-4 ZCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)



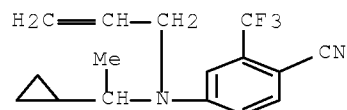
RN 821777-31-5 ZCAPLUS

CN Ethanone, 1-[4-[(cyclopropylmethyl)propylamino]-2-(trifluoromethyl)phenyl]-
(CA INDEX NAME)



RN 821777-33-7 ZCAPLUS

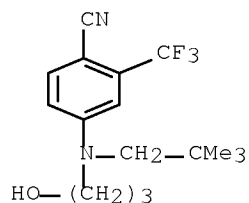
CN Benzonitrile, 4-[(1-cyclopropylethyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



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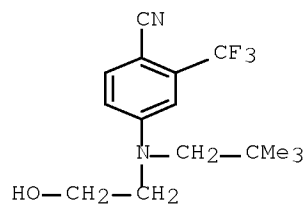
RN 821777-35-9 ZCAPLUS

CN Benzonitrile, 4-[(2,2-dimethylpropyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



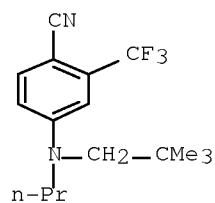
RN 821777-39-3 ZCAPLUS

CN Benzonitrile, 4-[(2,2-dimethylpropyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-40-6 ZCAPLUS

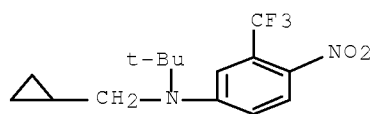
CN Benzonitrile, 4-[(2,2-dimethylpropyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-43-9 ZCAPLUS

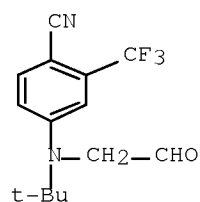
CN Benzenamine, N-(cyclopropylmethyl)-N-(1,1-dimethylethyl)-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)

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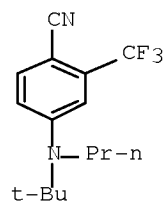
RN 821777-45-1 ZCAPLUS

CN Benzonitrile, 4-[(1,1-dimethylethyl)(2-oxoethyl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-46-2 ZCAPLUS

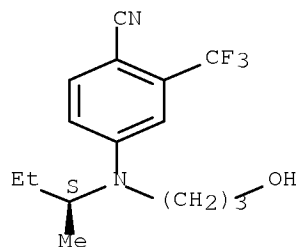
CN Benzonitrile, 4-[(1,1-dimethylethyl)propylamino]-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-47-3 ZCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)[(1S)-1-methylpropyl]amino]-2-(
(trifluoromethyl)- (CA INDEX NAME)

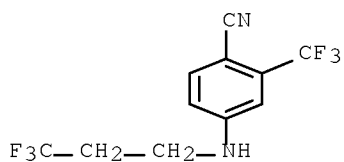
Absolute stereochemistry.



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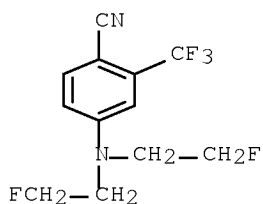
RN 821777-48-4 ZCAPLUS

CN Benzonitrile, 2-(trifluoromethyl)-4-[(3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)



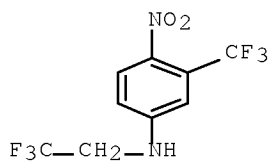
RN 821777-49-5 ZCAPLUS

CN Benzonitrile, 4-[bis(2-fluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



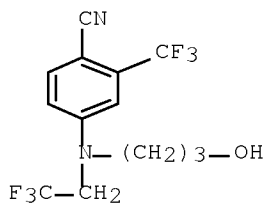
RN 821777-51-9 ZCAPLUS

CN Benzenamine, 4-nitro-N-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-52-0 ZCAPLUS

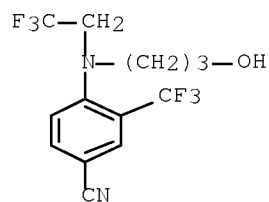
CN Benzonitrile, 4-[(3-hydroxypropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/560012

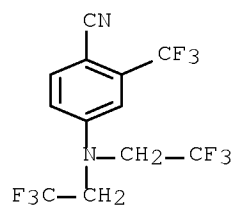
RN 821777-53-1 ZCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)(2,2,2-trifluoroethyl)amino]-3-(trifluoromethyl)- (CA INDEX NAME)



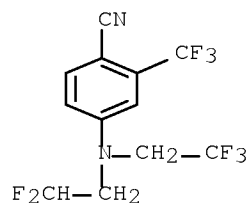
RN 821777-55-3 ZCAPLUS

CN Benzonitrile, 4-[bis(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-56-4 ZCAPLUS

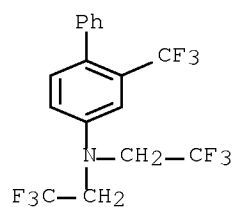
CN Benzonitrile, 4-[(2,2-difluoroethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-57-5 ZCAPLUS

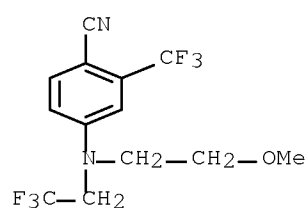
CN [1,1'-Biphenyl]-4-amine, N,N-bis(2,2,2-trifluoroethyl)-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



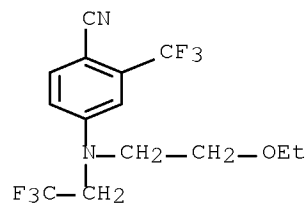
RN 821777-59-7 ZCAPLUS

CN Benzonitrile, 4-[(2-methoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



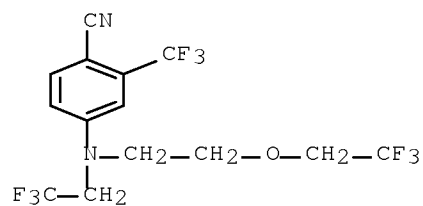
RN 821777-60-0 ZCAPLUS

CN Benzonitrile, 4-[(2-ethoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-61-1 ZCAPLUS

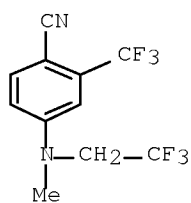
CN Benzonitrile, 4-[[2-(2,2,2-trifluoroethoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/560012

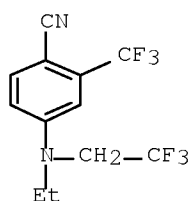
RN 821777-62-2 ZCAPLUS

CN Benzonitrile, 4-[methyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



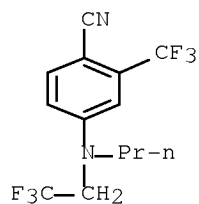
RN 821777-63-3 ZCAPLUS

CN Benzonitrile, 4-[ethyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-64-4 ZCAPLUS

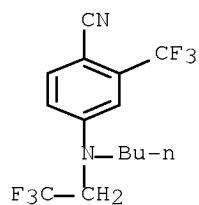
CN Benzonitrile, 4-[propyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)



RN 821777-65-5 ZCAPLUS

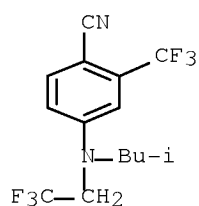
CN Benzonitrile, 4-[butyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-
(CA INDEX NAME)

10/560012



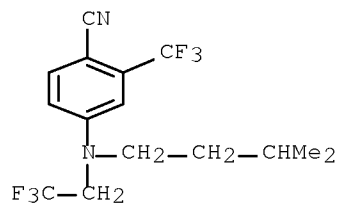
RN 821777-67-7 ZCAPLUS

CN Benzonitrile, 4-[(2-methylpropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



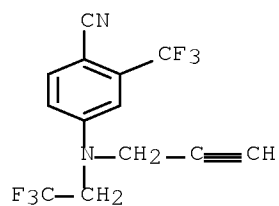
RN 821777-69-9 ZCAPLUS

CN Benzonitrile, 4-[(3-methylbutyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-70-2 ZCAPLUS

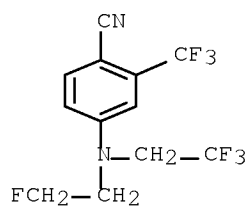
CN Benzonitrile, 4-[2-propyn-1-yl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



10/560012

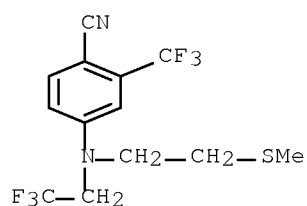
RN 821777-71-3 ZCAPLUS

CN Benzonitrile, 4-[(2-fluoroethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



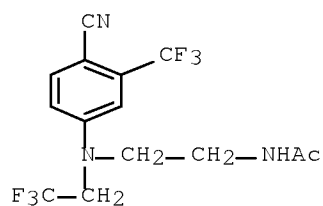
RN 821777-72-4 ZCAPLUS

CN Benzonitrile, 4-[[2-(methylthio)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



RN 821777-74-6 ZCAPLUS

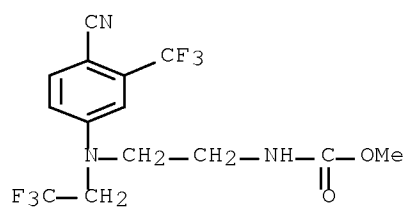
CN Acetamide, N-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)



RN 821777-75-7 ZCAPLUS

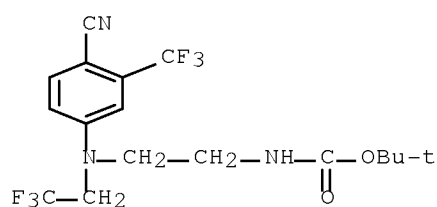
CN Carbamic acid, [2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

10/560012



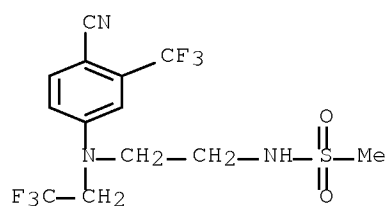
RN 821777-76-8 ZCAPLUS

CN Carbamic acid, [2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



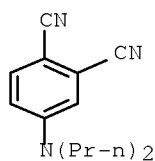
RN 821777-77-9 ZCAPLUS

CN Methanesulfonamide, N-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)



RN 821777-78-0 ZCAPLUS

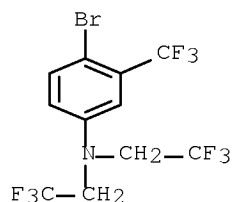
CN 1,2-Benzenedicarbonitrile, 4-(dipropylamino)- (CA INDEX NAME)



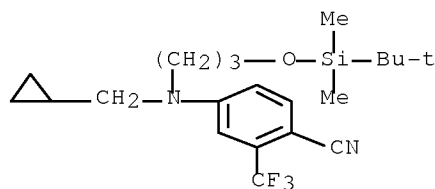
RN 821778-33-0 ZCAPLUS

10/560012

CN Benzenamine, 4-bromo-N,N-bis(2,2,2-trifluoroethyl)-3-(trifluoromethyl)-
(CA INDEX NAME)

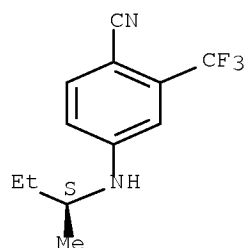


IT 821777-79-1P 821777-80-4P 821777-85-9P
821777-86-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of substituted anilines as androgen receptor modulators)
RN 821777-79-1 ZCAPLUS
CN Benzonitrile, 4-[(cyclopropylmethyl)[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]amino]-2-(trifluoromethyl)- (CA
INDEX NAME)



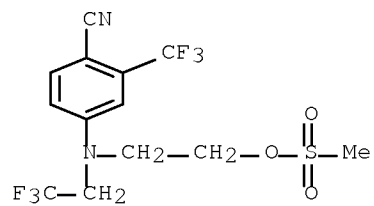
RN 821777-80-4 ZCAPLUS
CN Benzonitrile, 4-[[[(1S)-1-methylpropyl]amino]-2-(trifluoromethyl)- (CA
INDEX NAME)

Absolute stereochemistry.



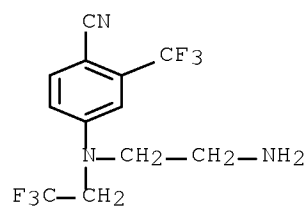
RN 821777-85-9 ZCAPLUS
CN Benzonitrile, 4-[[2-[(methylsulfonyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

10/560012



RN 821777-86-0 ZCAPLUS

CN Benzonitrile, 4-[(2-aminoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file registry

FILE 'REGISTRY' ENTERED AT 11:02:42 ON 12 MAR 2009

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DICTIONARY FILE UPDATES: 11 MAR 2009 HIGHEST RN 1119363-64-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

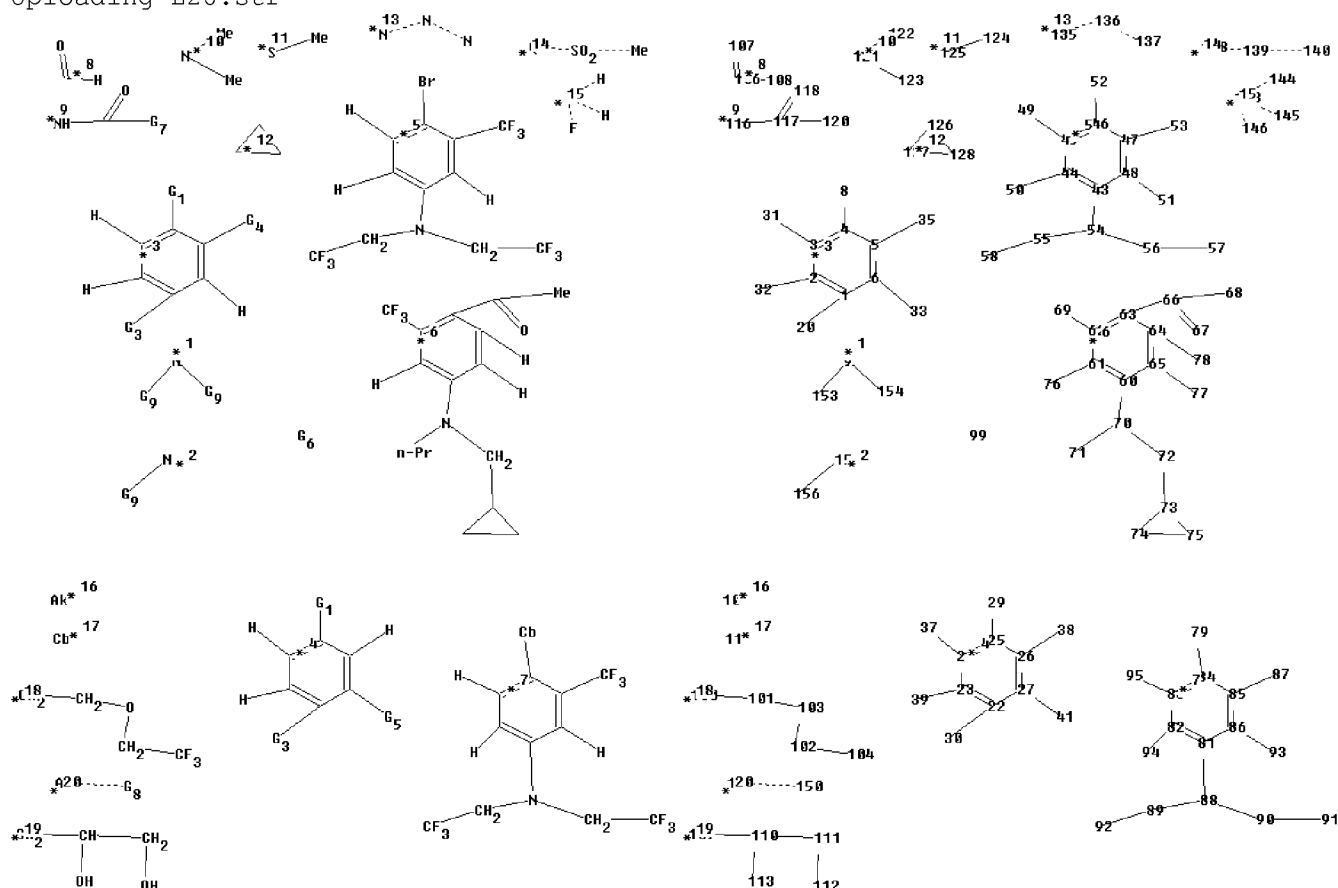
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

Uploading L26.str



10/560012

chain nodes :

8 9 10 11 15 20 29 30 31 32 33 35 37 38 39 41 49 50 51 52 53
54 55 56 57 58 66 67 68 69 70 71 72 76 77 78 79 87 88 89 90 91
92 93 94 95
99 100 101 102 103 104 106 107 108 109 110 111 112 113 115 116 117
118 120 121
122 123 124 125 135 136 137 138 139 140 143 144 145 146 150 153 154
156

ring nodes :

1 2 3 4 5 6 22 23 24 25 26 27 43 44 45 46 47 48 60 61 62 63
64 65 73 74 75 81 82 83 84 85 86 126 127 128

chain bonds :

1-20 2-32 3-31 4-8 5-35 6-33 9-153 9-154 15-156 22-30 23-39 24-37 25-29
26-38 27-41 43-54 44-50 45-49 46-52 47-53 48-51 54-55 54-56 55-58 56-57
60-70 61-76
62-69 63-66 64-78 65-77 66-67 66-68 70-71 70-72 72-73 79-84 81-88 82-94
83-95 85-87
86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108
106-107 109-110
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123
124-125 135-136
136-137 138-139 139-140 143-144 143-145 143-146

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75
74-75 81-82
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128

exact/norm bonds :

1-20 4-8 5-35 9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120
126-127 126-128
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146

exact bonds :

2-32 3-31 6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73
79-84 82-94 83-95
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-
108 109-110
110-111 111-112 121-122 121-123 124-125

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86
82-83 83-84
84-85 85-86

isolated ring systems :

containing 1 : 22 : 43 : 60 : 81 :

G1:CN,NO2

G3:[*1],[*2]

G4:CF3,C1,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,C1

G6:[*3],[*4],[*5],[*6],[*7]

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G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15]

G9:[*16],[*17],[*18],[*19],[*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain
125:2 E exact
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS
30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom
44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS
54:CLASS 55:CLASS
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom
66:CLASS
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom
75:Atom 76:CLASS 77:CLASS
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS
88:CLASS
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS
100:CLASS 101:CLASS
102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 111:CLASS
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS
121:CLASS 122:CLASS
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS
137:CLASS
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS
150:CLASS 153:CLASS
154:CLASS 156:CLASS

Generic attributes :

11:

Saturation : Saturated

79:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 10: Limited

C,C7

Node 11: Limited

C,C6

Node 79: Limited

C,C6

Node 115: Limited

C,C6

=> d stat que L70

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82177
L14      SCR 616
L26      STR
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L32      SCR 1840 OR 2043 OR 1951
L35      898352 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (N>1 AND ((46.150.18/
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D OR 46.150.1/RID) AND 2/NRS))) NOT PMS/CI
L38      1054 SEA FILE=REGISTRY SUB=L35 SSS FUL L26 AND ((L14 AND L27) NOT
L32)
L47      135 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L38 AND L3
L48      16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L3 NOT L47
L50      1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L48 AND BR/ELS AND
9/F
L51      10 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L48 NOT BR/ELS
L52      6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L51 AND F/ELS
L53      7 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L50 OR L52
L54      142 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L47 OR L53
L55      65815 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C14H19N3O2/MF OR
C13H17N3O2/MF OR C12H13F3N2/MF OR C13H12F6N2O/MF OR C13H13N3O2/
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 C14H14F6N2/MF OR C14H15F3N2O/MF OR C14H17F3N2/MF OR C14H17F3N2O
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 2/MF OR C16H21F3N2/MF OR C10H11F3N2O2/MF OR C10H11F3N2O3/MF OR
 C10H13CLN2O3/MF OR C10H6F6N2/MF OR C10H9F3N2/MF OR C11H11F3N2/M
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L59	19	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L57 NOT L58
L60	16	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L59 AND PY<2004
L61	28	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L58 AND PD<20030610
L62	35	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L58 AND PRD<20030610
L63	30	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L58 AND AD<20030610
L64	51	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON (L60 OR L61 OR L62 OR L63)
L66	142	SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L55 AND L54
L67	366	SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L56 OR L66
L68	68	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L67
L70	51	SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L68 AND L64

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 11:02:50 ON 12 MAR 2009

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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d ibib abs hitstr L70 1-51

L70 ANSWER 1 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1342415 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:89971
TITLE: Nile red luminescent compound emitting red light,
process for producing the same and luminescence
element utilizing the same
INVENTOR(S): Nakaya, Tadao; Tajima, Akio; Saikawa, Tomoyuki;
Takano, Shinji; Yamauchi, Takao; Mori, Hidemasa
PATENT ASSIGNEE(S): Hirose Engineering Co., Ltd, Japan
SOURCE: U.S. Pat. Appl. Publ., 55pp., Division of U.S. Ser.
No. 501,398.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287524	A1	20061221	US 2006-486111	20060831
US 20050113575	A1	20050526	US 2004-501398	20040715 <--
PRIORITY APPLN. INFO.:			US 2004-501398	A3 20040715
			JP 2002-12222	A 20020121 <--
			JP 2002-12224	A 20020121 <--
			JP 2002-14881	A 20020123 <--
			JP 2002-172127	A 20020612 <--
			WO 2003-JP477	W 20030121 <--

OTHER SOURCE(S): MARPAT 146:89971

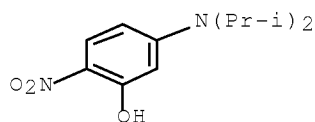
AB Luminescent derivs. of 9-amino-5H-benzo[a]phenoxazin-5-one (Nile Red derivs.) and methods for producing them are described. Electroluminescent devices employing the compds. are also described. The patent also describes the preparation of unclaimed luminescent derivs. of 9-amino-5H-benzo[a]phenothiazin-5-one.

IT ~~398482-49-0~~

RL: RCT (Reactant); RACT (Reactant or reagent)
(luminescent aminobenzophenoxazinone derivs. and their preparation and light-emitting devices using them)

RN 398482-49-0 ZCAPLUS

CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)



L70 ANSWER 2 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:902613 ZCAPLUS Full-text
 DOCUMENT NUMBER: 143:248160
 TITLE: Preparation of benzamides for promoting apoptosis
 INVENTOR(S): Bajji, Ashok C.; Arranz, Esther; Srinivasan, Jayasree
 M.; Delmar, Eric; Slade, Rachel; Willardsen, Jon Adam
 PATENT ASSIGNEE(S): Myriad Genetics, Incorporated, USA
 SOURCE: U.S. Pat. Appl. Publ., 121 pp., Cont.-in-part of Appl.
 No. PCT/US03/22183.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050187300	A1	20050825	US 2005-39275	20050118 <--
WO 2004006858	A2	20040122	WO 2003-US22183	20030715 <--
WO 2004006858	A3	20040429		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-396266P P 20020715 <--
 US 2002-396773P P 20020716 <--
 WO 2003-US22183 A2 20030715

OTHER SOURCE(S): CASREACT 143:248160; MARPAT 143:248160
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Benzamides, e.g. I (R2, R3 = halo, C1-C6-haloalkyl; R4, R5 = C1-C6-alkyl; R6 = H, halo; R7 = halo, C1-C4-haloalkyl) and II [R11, R12, R13, R14, R15, R16, R17, R18 = H, halo, N3, OH, SH, cyano, C1-C6-(halo)(hydroxy)alkyl, C2-C6-alkenyl, C2-C6-alkenyloxy, C2-C6-alkynyloxy, C1-C6-alkylsulfonamide, carbocycle, heterocyclyl, (hetero)aryl, NR50R51, NR50COR40, CONR50R51, C(:G1)G2R41, etc.; R40 = H, OH, C1-C6-alkyl, C2-C6-alkenyl, C2-C6-alkynyl, C1-C6-alkoxy, C2-C6-alkenyloxy, C2-C6-alkynyloxy, C1-C6-alkylthiol; R41 = H, C1-C6-alkyl, C2-C6-alkenyl, C2-C6-alkynyl; R50, R51 = H, OH, C1-C10-(halo)alkyl, C2-C10-alkenyl, C2-C10-alkynyl, C1-C10-alkoxy, C1-C10-alkylthiol, C2-C10-alkenyloxy, C2-C10-alkynyloxy, C2-C6-hydroxyalkyl, etc.; R19 = H, C1-C6-alkyl;

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R20 = haloalkyl, C2-C6-alkoxy, C2-C6-alkyl, alkylene-O-R8, alkylene-R8, alkylene(R8R9), alkylene = C1-C6-alkylene, R8, R9 = cycloalkyl, aryl, heterocyclyl, heteroaryl; Z = O, NR21, S, R21 = H, C1-C6-alkyl], were prepared to promote apoptosis. To illustrate the synthesis, reacting 3-O2NC6H4OH with PhCH2CH2OH gave 3-O2NC6H4OCH2CH2Ph which was reduced to the amine and acylated with 5-chlorosalicylic acid to give benzamide III.

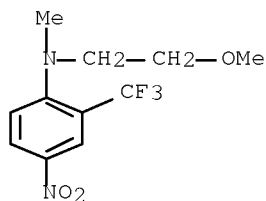
IT 821777-13-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzamide derivs. for promoting apoptosis)

RN 821777-13-3 ZCAPLUS

CN Benzenamine, N-(2-methoxyethyl)-N-methyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 3 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:802711 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:314020

TITLE: Preparation of substituted p-diaminobenzene derivatives as openers of the KCNQ family potassium ion channels

INVENTOR(S): Khanzhin, Nikolay; Rottlaender, Mario; Ritzen, Andreas; Watson, William Patrick

PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.

SOURCE: PCT Int. Appl., 176 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

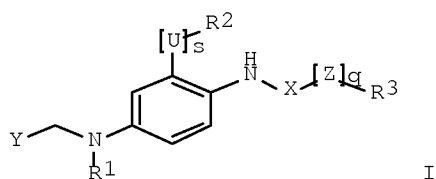
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004082677	A1	20040930	WO 2004-DK186	20040318 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004222626	A1	20040930	AU 2004-222626	20040318 <--
CA 2519582	A1	20040930	CA 2004-2519582	20040318 <--

10/560012

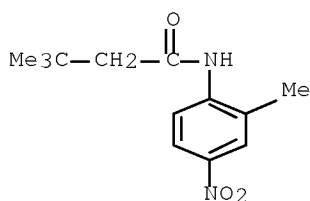
EP 1613303 A1 20060111 EP 2004-721472 20040318 <--
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK
 BR 2004008437 A 20060404 BR 2004-8437 20040318 <--
 CN 1761464 A 20060419 CN 2004-80007507 20040318 <--
 JP 2006520759 T 20060914 JP 2006-504330 20040318 <--
 IN 2005CN02347 A 20070831 IN 2005-CN2347 20050921 <--
 NO 2005004848 A 20051020 NO 2005-4848 20051020 <--
 US 20060183791 A1 20060817 US 2005-550448 20051116 <--
 PRIORITY APPLN. INFO.: DK 2003-441 A 20030321 <--
 US 2003-456698P P 20030321 <--
 WO 2004-DK186 W 20040318
 OTHER SOURCE(S): CASREACT 141:314020; MARPAT 141:314020
 GI



AB The title anilines I [s = 0-1; U = O, S, SO2, etc.; q = 0-1; X = CO, SO2; with the proviso that q = 0 when X = SO2; Z = O, S; R1 = H, alk(en/yn)yl, cycloalk(en)yl, etc.; R2 = H, alk(en/yn)yl, cycloalk(en)yl, etc.; R3 = alk(en/yn)yl, cycloalk(en)yl, heterocycloalk(en)yl, etc.; Y = (un)substituted Ph, naphthyl, thienyl, etc.], useful for the prevention, treatment or inhibition of a disorder being responsive to an increased ion flow in a potassium channel, were prepared and formulated. Thus, reductive amination of Pr (4-amino-2-methylphenyl)carbamate (preparation given) with benzofuran-2-carbaldehyde in the presence of NaBH3CN afforded 43% Pr {4-[(benzofuran-2-ylmethyl)amino]-2-methylphenyl}carbamate. The compds. I have an EC50 of <20000nM, in most cases <2000nM and in many cases <200nM in KCNQ2 channel assay.

IT 335204-56-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of substituted p-diaminobenzene derivs. as openers of the KCNQ family potassium ion channels)

RN 335204-56-3 ZCAPLUS
 CN Butanamide, 3,3-dimethyl-N-(2-methyl-4-nitrophenyl)- (CA INDEX NAME)



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REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 4 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:430796 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:7139

TITLE: Preparation of indolylquinoxalinones for treating
hyperproliferative disorders and diseases associated
with angiogenesis

INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng;
Brittelli, David R.; Burke, Michael J.; Chen, Gang;
Cook, James; Dumas, Jacques; Sibley, Robert; Turner,
Michael R.

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: ~~Patent~~

LANGUAGE: English

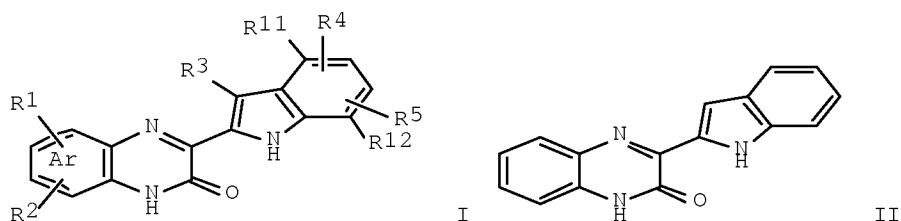
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004043950	A1	20040527	WO 2003-US36003	20031110 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,				
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,				
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,				
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,				
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,				
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,				
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2505819	A1	20040527	CA 2003-2505819	20031110 <--
AU 2003290744	A1	20040603	AU 2003-290744	20031110 <--
EP 1565455	A1	20050824	EP 2003-783328	20031110 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016169	A	20050927	BR 2003-16169	20031110 <--
CN 1738814	A	20060222	CN 2003-80108639	20031110 <--
JP 2006509840	T	20060323	JP 2005-507146	20031110 <--
MX 2005004779	A	20050722	MX 2005-4779	20050504 <--
US 20060004011	A1	20060105	US 2005-534215	20050506
NO 2005002796	A	20050609	NO 2005-2796	20050609 <--
PRIORITY APPLN. INFO.:			US 2002-425490P	P 20021112 <--
			US 2003-460915P	P 20030407 <--
			US 2003-484202P	P 20030630
			WO 2003-US36003	W 20031110

OTHER SOURCE(S): MARPAT 141:7139

GI



AB The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF₃, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO₂, NH₂, alkylamino, alkoxyamino, or (un)substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%).

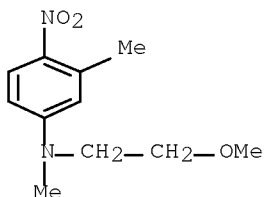
IT 694533-16-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

RN 694533-16-9 ZCAPLUS

CN Benzenamine, N-(2-methoxyethyl)-N,3-dimethyl-4-nitro- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 5 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:287838 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:321373

TITLE: Preparation of novel pyrimidine amides as protein kinase inhibitors

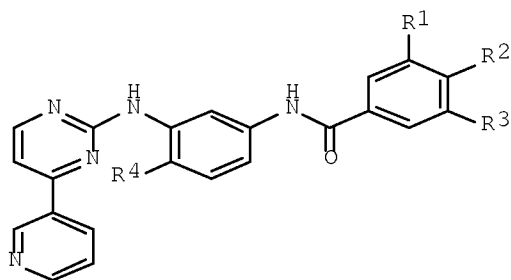
INVENTOR(S): Manley, Paul William; Breitenstein, Werner; Jacob,

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Sandra; Furet, Pascal
 PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH
 SOURCE: PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029038	A1	20040408	WO 2003-EP10724	20030926 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2499822	A1	20040408	CA 2003-2499822	20030926 <--
AU 2003270277	A1	20040419	AU 2003-270277	20030926 <--
AU 2003270277	B2	20070823		
EP 1546127	A1	20050629	EP 2003-750639	20030926 <--
EP 1546127	B1	20070808		
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BR 2003014797	A	20050726	BR 2003-14797	20030926 <--
CN 1684951	A	20051019	CN 2003-823213	20030926 <--
CN 100404528	C	20080723		
JP 2006508064	T	20060309	JP 2004-539039	20030926 <--
AT 369355	T	20070815	AT 2003-750639	20030926 <--
ES 2288615	T3	20080116	ES 2003-750639	20030926 <--
NZ 538930	A	20080430	NZ 2003-538930	20030926 <--
ZA 2005002304	A	20060426	ZA 2005-2304	20050318 <--
MX 2005003253	A	20050608	MX 2005-3253	20050323 <--
IN 2005CN00464	A	20070406	IN 2005-CN464	20050323 <--
KR 876055	B1	20081226	KR 2005-705204	20050325 <--
NO 2005001966	A	20050422	NO 2005-1966	20050422 <--
HK 1080459	A1	20080215	HK 2005-111972	20051223 <--
US 20060142577	A1	20060629	US 2006-528913	20060105 <--
KR 2007098940	A	20071005	KR 2007-719251	20070823 <--
IN 2007CN04330	A	20080125	IN 2007-CN4330	20071001 <--
PRIORITY APPLN. INFO.:			GB 2002-22514	A 20020927 <--
			WO 2003-EP10724	W 20030926
			IN 2005-CN464	A3 20050323
			KR 2005-705204	A3 20050325

OTHER SOURCE(S): MARPAT 140:321373
 GI



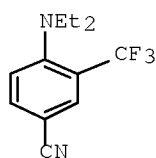
I

AB The title substituted N-(3-benzoylamino-phenyl)-4-pyridyl-2-pyrimidinamines [I; R1 = H and R2 = NR5R6, or R1 = NR5R6 and R2 = H; R3 = alkyl, fluoroalkyl, hydroxyalkyl, carbamoyl; R4 = H, alkyl, halo; R5 and R6 = H, alkyl, hydroxyalkyl, etc. or NR5R6 = (un)substituted (un)saturated 5-7 membered ring optionally containing heteroatoms], useful for the therapy of a disease which responds to an inhibition of protein kinase activity, especially a neoplastic disease (e.g., leukemia), were prepared and formulated. Thus, amidation of 4-methyl-N-[4-(3-pyridinyl)-2-pyrimidinyl]-1,3-benzenediamine with 4-diethylamino-3-(trifluoromethyl)benzoic acid (preparation given) afforded I [R1 = H; R2 = NEt2; R3 = CF3; R4 = Me] which showed IC50 of 50-100 nM against c-Abl and IC50 of 200-500 nM against Bcr-Abl (in vitro inhibition data).

IT 677704-53-9P, 4-(Diethylamino)-3-(trifluoromethyl)benzonitrile
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of novel N-[3-(pyrimidin-2-ylamino)phenyl] benzamides as protein kinase inhibitors)

RN 677704-53-9 ZCAPLUS

CN Benzonitrile, 4-(diethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

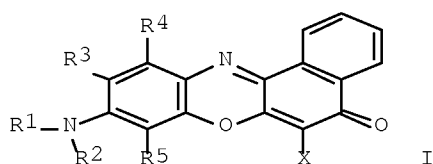
L70 ANSWER 6 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:591159 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:157136
 TITLE: Nile red type compound emitting red light, process for producing the same, and luminescent element utilizing the same
 INVENTOR(S): Nakaya, Tadao; Tajima, Akio; Saikawa, Tomoyuki; Takano, Shinji; Yamauchi, Takao; Mori, Hidemasa
 PATENT ASSIGNEE(S): Taiho Industries, Co. Ltd., Japan
 SOURCE: PCT Int. Appl., 112 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese

10/560012

FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062213	A1	20030731	WO 2003-JP477	20030121 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2003277371	A	20031002	JP 2002-14881	20020123 <--
JP 2004018400	A	20040122	JP 2002-172127	20020612 <--
JP 2003277369	A	20031002	JP 2003-12498	20030121 <--
EP 1475372	A1	20041110	EP 2003-701142	20030121 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1620441	A	20050525	CN 2003-802508	20030121 <--
US 20050113575	A1	20050526	US 2004-501398	20040715 <--
PRIORITY APPLN. INFO.:			JP 2002-12222	A 20020121 <--
			JP 2002-12224	A 20020121 <--
			JP 2002-14881	A 20020123 <--
			JP 2002-172127	A 20020612 <--
			JP 2001-313245	A 20011010 <--
			WO 2003-JP477	W 20030121 <--

OTHER SOURCE(S): MARPAT 139:157136
GI



AB The invention relates to a Nile red-based red-emitting compound represented by I [R1-2 = H and alkyl; R3(R5) = H and may combine with R1(R2) to form a ring; R4 = H and may combine with R3 to form a ring; X = H, halo, and -CH(CN)Ar]. The compound is suited for use as a red-emitting material in an organic light emitting device.

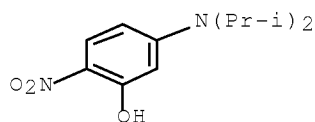
IT 398482-49-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(nile red type compound for red-emitting organic LED)

RN 398482-49-0 ZCAPLUS

CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)

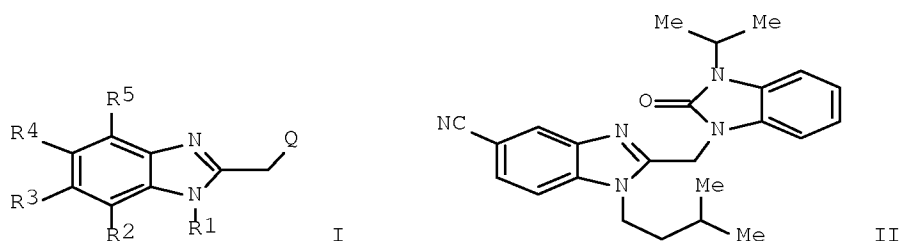
10/560012



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 7 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:511082 ZCAPLUS Full-text
 DOCUMENT NUMBER: 139:85343
 TITLE: Preparation of 2-(heterocyclylmethyl)benzimidazoles as respiratory syncytial virus antiviral agents
 INVENTOR(S): Yu, Kuo-long; Wang, Xiangdong; Sun, Yaxiong; Cianci, Christopher; Thuring, Jan Willem; Combrink, Keith; Meanwell, Nicholas; Zhang, Yi; Civiello, Rita L.
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 149 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053344	A2	20030703	WO 2002-US39220	20021206 <--
WO 2003053344	A3	20031113		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20030207868	A1	20031106	US 2002-309505	20021204 <--
US 6919331	B2	20050719		
AU 2002362094	A1	20030709	AU 2002-362094	20021206 <--
EP 1461035	A2	20040929	EP 2002-797226	20021206 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRIORITY APPLN. INFO.:			US 2001-339025P	P 20011210 <--
			WO 2002-US39220	W 20021206 <--
OTHER SOURCE(S):			MARPAT 139:85343	
GI				



AB Title compds. I [wherein R1 = (CRaRb)_nX; R2 = H; R3 = CONRhRi, CO2Rd, or (un)substituted alkyl; R4 = NH2, CONRhRi, heteroaryl, alkenyl, CO2Rd, N=CPh2, C(NOH)NH2, C(NH)NH2, or (un)substituted alkyl; R5 = CO2Rj or (un)substituted alkyl or alkenyl; Q = (un)substituted benzimidazolyl, benzotriazolyl, imidazopyridinyl, quinolinyl, quinazolinyl, benzyloxy, etc.; X = H or (un)substituted alkyl; Ra and Rb = independently H or (halo)alkyl; Rd = alkyl; Rh and Ri = independently H or alkyl; Rj = H or alkyl; n = 1-6; and pharmaceutically acceptable salts thereof] were prepared as antiviral compds. More particularly, the invention provides 2-(heterocyclylmethyl)benzimidazole derivs. for the treatment of respiratory syncytial virus (RSV) infection. For example, 1-isopropyl-1,3-dihydrobenzimidazol-2-one was coupled with 2-chloromethyl-1-(3-methylbutyl)-1H-benzimidazole-5-carbonitrile in the presence of Cs2CO3 in DMF to give II (95%). Disclosed compds. protected HEp-2 cells from RSV-induced cytopathic effects with EC50 values between 50 μM and 0.001 μM, compared to an EC50 of 3 μM for ribavirin. I also displayed antiviral activity by reducing viral protein expression in HEp-2 cells with EC50 values between 50 μM and 0.001 μM, compared to an EC50 value of 3 μM for ribavirin. Thus, I and compns. comprising I are useful for the treatment of RSV infections.

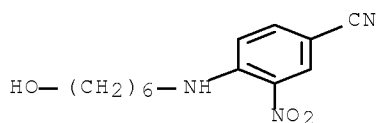
IT 554457-74-8P 554458-11-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of (heterocyclylmethyl)benzimidazoles as RSV antiviral agents)

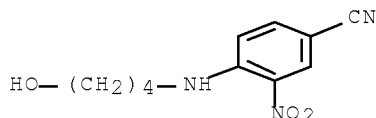
RN 554457-74-8 ZCAPLUS

CN Benzonitrile, 4-[(6-hydroxyhexyl)amino]-3-nitro- (CA INDEX NAME)



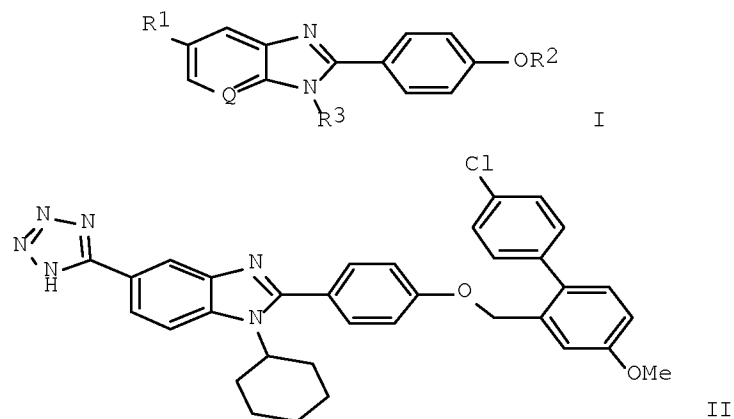
RN 554458-11-6 ZCAPLUS

CN Benzonitrile, 4-[(4-hydroxybutyl)amino]-3-nitro- (CA INDEX NAME)



L70 ANSWER 8 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:261620 ZCAPLUS Full-text
 DOCUMENT NUMBER: 138:287673
 TITLE: Preparation of phenylbenzimidazole compounds useful
 for treating hepatitis C virus
 INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,
 Thomas W.; Zheng, Xiaofan
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 74 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926 <--
WO 2003026587	A3	20031106		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002337765	A1	20030407	AU 2002-337765	20020926 <--
US 20030134853	A1	20030717	US 2002-259041	20020926 <--
EP 1429759	A2	20040623	EP 2002-773657	20020926 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
US 20040067976	A1	20040408	US 2003-648873	20030827 <--
US 6803374	B2	20041012		
PRIORITY APPLN. INFO.:			US 2001-324874P	P 20010926 <--
			US 2002-259041	B1 20020926 <--
			WO 2002-US30989	W 20020926 <--
OTHER SOURCE(S):	MARPAT 138:287673			
GI				



AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO₂, PhCONHSO₂, etc.; R2 = CH₂-aryl, CHPh₂, etc.; R3 = cycloalkyl] are prepared which are useful in treating viral hepatitis C. Thus, II was prepared and had an IC₅₀ of 0.14 μM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

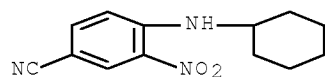
IT 28096-55-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 28096-55-1 ZCAPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



L70 ANSWER 9 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:418358 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:370024

TITLE: Synthesis of some new 2-substituted-phenyl-1H-benzimidazole-5-carbonitriles and their potent activity against Candida species

AUTHOR(S): Goker, Hakan; Kus, Canan; Boykin, David W.; Yildiz, Sulhiye; Altanlar, Nurten

CORPORATE SOURCE: Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara University, Ankara, 06100, Turk.

SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(8), 2589-2596

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:370024

AB New 2-substituted-phenyl-1H-benzimidazole-5-carboxylic acids, ethyl-5-carboxylate, -5-carboxamides, -5-carboxaldehyde, -5-chloro-, -5-

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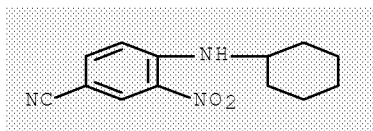
trifluoromethyl, and -5-carbonitriles, -6-carbonitrile were prepared and evaluated in vitro against Candida species. The cyano substituted compds. exhibited the greatest activity with MIC values of 3.12 µg/mL, values similar to that of fluconazole.

IT 28096-55-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and m.p. of 2-substituted-Ph-1H-benzimidazole-5-carbonitriles)

RN 28096-55-1 ZCAPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 10 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:122974 ZCAPLUS Full-text

DOCUMENT NUMBER: 136:191436

TITLE: Nile-red luminescent compound, process for producing the same, and luminescent element utilizing the same

INVENTOR(S): Nakaya, Tadao; Yamauchi, Takao; Saikawa, Tomoyuki; Tajima, Akio; Mori, Hidemasa

PATENT ASSIGNEE(S): Taiho Industries, Co., Ltd, Japan

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

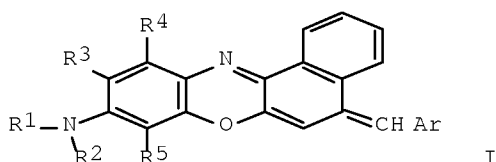
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002012208	A1	20020214	WO 2001-JP5671	20010629 <--
W: CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 20040054174	A1	20040318	US 2003-416586	20030513 <--
PRIORITY APPLN. INFO.:			JP 2000-236670	A 20000804 <--
			JP 2000-348516	A 20001115 <--
			WO 2001-JP5671	W 20010629 <--

OTHER SOURCE(S): MARPAT 136:191436

GI

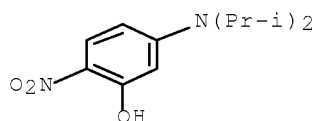


AB The invention provides a novel nile-red compound capable of emitting a nearly crimson red light; a novel process for producing the compound; and a luminescent compound which emits a nearly crimson red color at a high luminance. The nile-red luminescent compound is obtained by converting C=O in a nile-red compound into C=CH-Ar (wherein Ar is a fluorinated aromatic group) and incorporating an electron-donating group into the nile-red skeleton. The novel production process comprises reacting a nile-red dye with an electron-attracting aromatic MeCN. The nile-red based luminescent composition comprises a nile-red luminescent compound represented by I [R1 = R2 = C1-5 alkyl; R3 = H, or may be combined with R1 to form -CH2CH2-CR6R7- [R6 = R7 = H, and C1-5 alkyl, where the carbon in -CR6R7- is joined to the benzene ring]; R4 = H or may be combined with R3 to form naphthalene ring; R5 = H or may be combined with R2 to form -CH2CH2-CR8R9- [R8 = R9 = H and C1-5 alkyl, where the carbon in -CR8R9- is joined to the benzene ring]; Ar = fluorinated aroms.].

IT 398482-49-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (production of nile-red luminescent compound for electroluminescent device)

RN 398482-49-0 ZCAPLUS

CN Phenol, 5-[bis(1-methylethyl)amino]-2-nitro- (CA INDEX NAME)



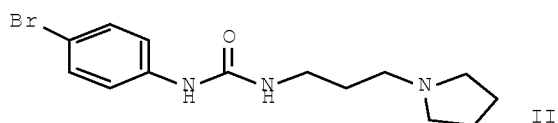
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 11 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:338479 ZCAPLUS Full-text
 DOCUMENT NUMBER: 134:353175
 TITLE: Preparation of amides and ureas as activators of soluble guanylate cyclase
 INVENTOR(S): Selwood, David; Glen, Robert; Reynolds, Karen; Wishart, Grant
 PATENT ASSIGNEE(S): University College London, UK
 SOURCE: PCT Int. Appl., 101 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032604	A1	20010510	WO 2000-GB4249	20001106 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				

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DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2389773 A1 20010510 CA 2000-2389773 20001106 <--
EP 1237849 A1 20020911 EP 2000-973061 20001106 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2003513064 T 20030408 JP 2001-534758 20001106 <--
PRIORITY APPLN. INFO.: GB 1999-26286 A 19991105 <--
US 2000-201382P P 20000502 <--
WO 2000-GB4249 W 20001106 <--
OTHER SOURCE(S): MARPAT 134:353175
GI



AB The title compds. R4PZNR1R2 [I; R1, R2 = alkyl; R1R2 together form alkylene; Z = alkylene; P = a direct bond, X, Y, W, XY, YW, XYW (wherein W = O, S, NR3; R3 = H, alkyl; Y = UV; V = a direct bond, alkylene; U = CS, CO, SO2, C(:NR); R = H, OH, alkyl; X = O, NR6; R6 = H, alkyl, alkenyl, etc.); R4 = alkyl, alkenyl, alkynyl, etc.], useful in the activation of soluble guanylate cyclase, were prepared E.g., synthesis of the urea II, starting with 4-bromoaniline and 1-(3-aminopropyl)pyrrolidine, was given. Biol. data for compds. I (e.g., IC50 for inhibition of platelet aggregation) were presented.

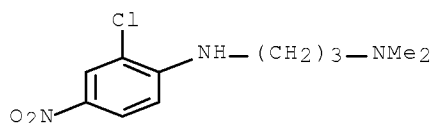
IT 338981-22-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amides and ureas as activators of soluble guanylate cyclase)

RN 338981-22-9 ZCAPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 12 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:63979 ZCAPLUS Full-text

DOCUMENT NUMBER: 134:100871

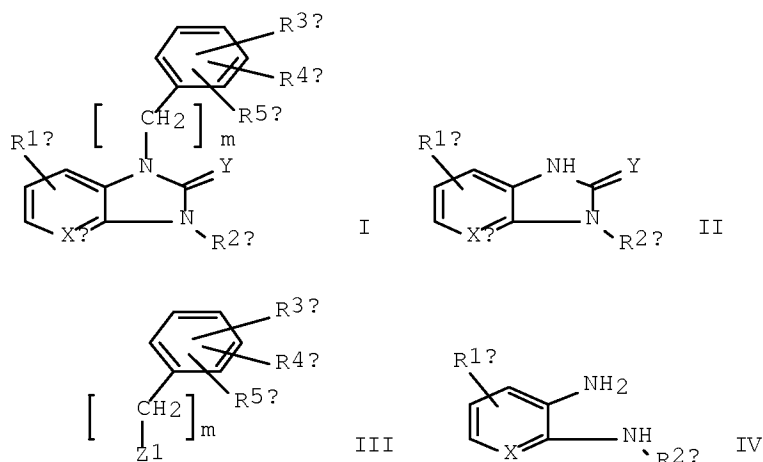
TITLE: Benzimidazolone derivatives, method of preparation and their use as phosphodiesterase inhibitors

INVENTOR(S): Sawada, Kozo; Inoue, Takayuki; Sawada, Yuki; Mizutani,

10/560012

PATENT ASSIGNEE(S): Tsuyoshi
 SOURCE: Fujisawa Pharmaceutical Co., Ltd., Japan
 PCT Int. Appl., 159 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005770	A1	20010125	WO 2000-JP4687	20000712 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2379554	A1	20010125	CA 2000-2379554	20000712 <--
AU 2000058531	A	20010205	AU 2000-58531	20000712 <--
EP 1196391	A1	20020417	EP 2000-944421	20000712 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200200161	T2	20020521	TR 2002-161	20000712 <--
BR 2000013041	A	20020716	BR 2000-13041	20000712 <--
HU 2002002186	A2	20021228	HU 2002-2186	20000712 <--
HU 2002002186	A3	20030228		
JP 2003505376	T	20030212	JP 2001-511431	20000712 <--
ZA 2002000029	A	20030402	ZA 2002-29	20020102 <--
IN 2002KN00019	A	20050311	IN 2002-KN19	20020103 <--
MX 2002000340	A	20020621	MX 2002-340	20020109 <--
US 6582351	B1	20030624	US 2002-30979	20020116 <--
PRIORITY APPLN. INFO.:			AU 1999-1747	A 19990721 <--
			AU 1999-2730	A 19990909 <--
			WO 2000-JP4687	W 20000712 <--
OTHER SOURCE(S):			MARPAT 134:100871	
GI				



AB Benzimidazolone derivs. I, its prodrugs or pharmaceutically acceptable salts thereof, a method for their preparation, pharmaceutical compns. containing them, and usefulness in treatment or prevention of diseases mediated by cyclic guanosine-3',5'-monophosphate phosphodiesterase (cGMP-PDE) are claimed. In I, Xa = CH or N; ya = O, S; R1a = halogen, cyano, NO2 carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, lower alkyl, halo(lower)alkyl, lower alkoxy, acyl, lower alkanesulfonyl. R2a = lower alkyl, cycloalkyl or heterocyclic group, among which the lower alkyl group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, lower alkylamino, acylamino, lower alkoxy-carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower alkanesulfonyl, lower alkylenedioxy, carbamoyl, lower alkyl carbamoyl and sulfamoyl; and the cycloalkyl group and the heterocyclic group may have 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy-carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl. R3a, R4a and R5a = same or different, H, halogen, lower alkanoyl, carboxy, protected carboxy, carbamoyl, nitro, cyano, lower alkyl optionally substituted by hydroxy, lower alkoxy or lower-alkoxy-substituted aralkyl; or two of R3a, R4a and R5a may combine together to form a lower alkylenedioxy. M = 1, 2, provided that when R3a = H, R4a = lower alkoxy and R5a = H, halogen, cyano, lower alkyl, lower alkoxy, protected carboxy, carboxy or nitro, then (1) the lower alkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy-carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, carboxy, lower alkanesulfonyl, lower alkylenedioxy, carbamoyl, lower alkyl carbamoyl and sulfamoyl, (2) the cycloalkyl for R2a has 1-3 substituents = OH, protected OH, acyl, lower-alkoxy-substituted aralkyloxy, amino, acylamino, lower alkoxy-carbonylamino, lower alkanesulfonylamino, ureido, lower alkylureido, sulfamoylamino, protected carboxy, lower alkanesulfonyl, lower alkyl, hydroxy(lower)alkyl, protected hydroxy(lower)alkyl, lower alkylenedioxy, carbamoyl and sulfamoyl, (3) the heterocyclic group for R2a = pyrrolidinyl, dioxanyl and piperidyl which groups may be substituted with protected carboxy, acyl, lower alkanesulfonyl, carbamoyl or sulfamoyl, (4) R1a = carbamoyl, lower alkylcarbamoyl which may be substituted with a heterocyclic group, carboxy, protected carboxy, acyl, or lower alkanesulfonyl, (5) Xa = N; (6) m = 2; or

(7) yra = S. Pharmaceutical compns. containing the above compds. are claimed (with test data provided for 8 compds.) to be effective for treatment or prevention of diseases mediated by cGMP-PDE: angina, hypertension, pulmonary hypertension, congestive heart failure, glomerular diseases, renal tubulointestinal diseases, renal failure, atherosclerosis, conditions of reduced blood vessel patency, peripheral vascular disease, stroke, bronchitis, asthma, allergic rhinitis, urticaria, glaucoma, diseases characterized by disorders of gut motility, erectile dysfunction, female sexual dysfunction, impotence, diabetic complications, micturition disorder, or incontinence and storage of urine disorder. The method of preparation comprises reacting II with III (Z1 = halogen) in the presence of base. III are made by intramol. cyclization of IV (X = N). For example, to a solution of 1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (200 mg) in anhydrous DMF (2 mL) was added portionwise NaH (29.3 mg, 60% dispersion in mineral oil) at 5° under N₂ atmosphere, and the mixture was stirred at room temperature for 30 min. After adding 3,4-dimethoxybenzyl bromide (154 mg), the mixture was stirred at room temperature for 2 h. After workup, 3-(3,4-dimethoxybenzyl)-1-(trans-4-hydroxycyclohexyl)-5-trifluoromethyl-2,3-dihydro-1H-benzimidazol-2-one (217.9 mg) was obtained as a colorless solid.

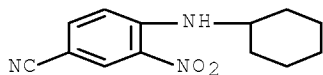
IT 28096-55-1P, 4-Cyclohexylamino-3-nitrobenzonitrile
 320405-95-6P, 4-[(1,1-Dimethyl-2-hydroxyethylamino)-3-nitrobenzonitrile 320406-03-9P,
 4-[(S)-1-Ethyl-2-hydroxyethylamino]-3-nitrobenzonitrile
 320406-04-0P, 4-[(R)-1-Ethyl-2-hydroxyethylamino]-3-nitrobenzonitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; benzimidazolone derivs., method of preparation and use as phosphodiesterase inhibitors)

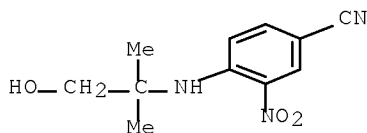
RN 28096-55-1 ZCAPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



RN 320405-95-6 ZCAPLUS

CN Benzonitrile, 4-[(2-hydroxy-1,1-dimethylethylamino)-3-nitro- (CA INDEX NAME)

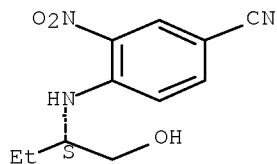


RN 320406-03-9 ZCAPLUS

CN Benzonitrile, 4-[(1S)-1-(hydroxymethyl)propylamino]-3-nitro- (CA INDEX NAME)

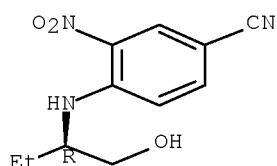
Absolute stereochemistry.

10/560012



RN 320406-04-0 ZCAPLUS
CN Benzonitrile, 4-[[1(1R)-1-(hydroxymethyl)propyl]amino]-3-nitro- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 13 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:401817 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:30667
TITLE: Heteroaryl-containing thiourea derivatives useful as inhibitors of herpes viruses
INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara, Bryan Mark
PATENT ASSIGNEE(S): American Home Products Corporation, USA
SOURCE: PCT Int. Appl., 164 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034269	A1	20000615	WO 1999-US28892	19991206 <--
W:			AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW	
RW:			GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG	
US 6166028	A	20001226	US 1999-444782	19991122 <--
US 6197803	B1	20010306	US 1999-447006	19991122 <--

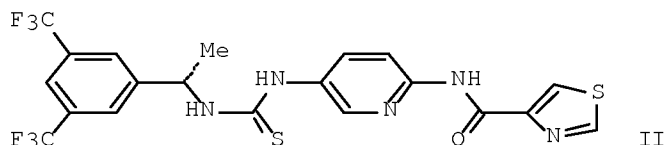
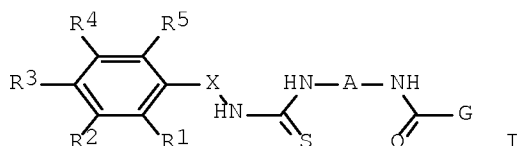
10/560012

US 6201013	B1	20010313	US 1999-444075	19991122 <--
CA 2351390	A1	20000615	CA 1999-2351390	19991206 <--
EP 1140913	A1	20011010	EP 1999-965143	19991206 <--
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BR 9916042	A	20011204	BR 1999-16042	19991206 <--
HU 2001004758	A2	20020429	HU 2001-4758	19991206 <--
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JP 2002531558	T	20020924	JP 2000-586716	19991206 <--
AU 756043	B2	20030102	AU 2000-31122	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
US 6271236	B1	20010807	US 2000-669943	20000926 <--
ZA 2001004373	A	20020918	ZA 2001-4373	20010528 <--
NO 2001002836	A	20010808	NO 2001-2836	20010608 <--
MX 2001005827	A	20010911	MX 2001-5827	20010608 <--
BG 105580	A	20020131	BG 2001-105580	20010608 <--
IN 2001KN00865	A	20050311	IN 2001-KN865	20010822 <--
IN 2001KN00866	A	20050311	IN 2001-KN866	20010822 <--
IN 2001KN00868	A	20050311	IN 2001-KN868	20010823 <--
US 20030036653	A1	20030220	US 2002-99695	20020315 <--
US 6555561	B2	20030429		

PRIORITY APPLN. INFO.:

US 1998-208540	A	19981209 <--
US 1998-150692P	P	19981209 <--
US 1998-150698P	P	19981209 <--
US 1998-155192P	P	19981209 <--
US 1998-155240P	P	19981209 <--
US 1998-208164	A	19981209 <--
US 1998-208559	A	19981209 <--
US 1998-208561	A	19981209 <--
US 1999-444782	A3	19991122 <--
WO 1999-US28892	W	19991206 <--
US 2000-669535	A3	20000926 <--
IN 2001-KN492	A3	20010508 <--
IN 2001-KN541	A3	20010522 <--
IN 2001-KN558	A3	20010525 <--

OTHER SOURCE(S): MARPAT 133:30667
GI



10/560012

AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; A = heteroaryl; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = aryl or heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 25 compds. in 2-4 bioassays. For instance, the pyridinylthiazolecarboxamide derivative II had an IC50 of 0.001 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.

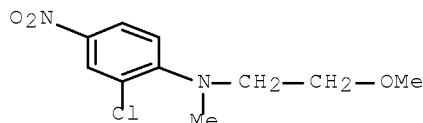
IT 151951-35-8 338981-22-9 821776-85-6
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Heteroaryl-containing thiourea derivatives useful as inhibitors of herpes viruses)

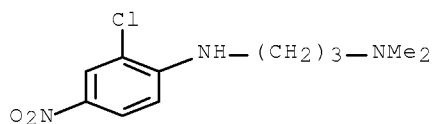
RN 151951-35-8 ZCAPLUS

CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



RN 338981-22-9 ZCAPLUS

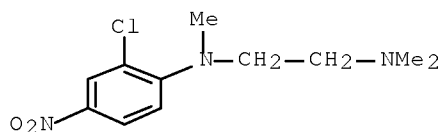
CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



RN 821776-85-6 ZCAPLUS

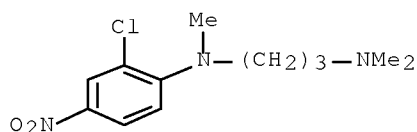
CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)

10/560012



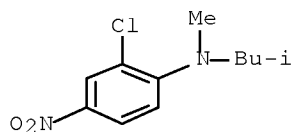
RN 821777-03-1 ZCAPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

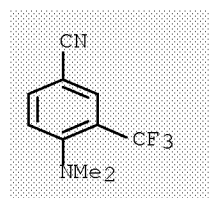
(starting material; preparation of heteroaryl-containing thiourea derivs.

as

inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/560012

L70 ANSWER 14 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401816 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:30666

TITLE: Aryl- and heteroaryl-substituted thiourea derivatives
useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph;
Dushin, Russell George; Lang, Stanley Albert; O'Hara,
Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

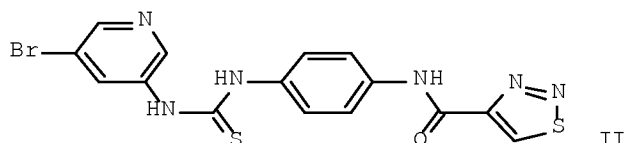
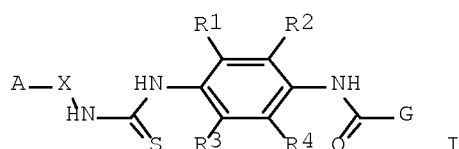
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

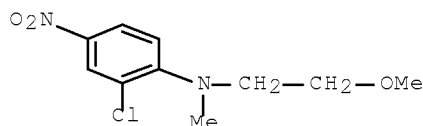
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034268	A1	20000615	WO 1999-US28838	19991206 <--
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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BR 9915993	A	20010904	BR 1999-15993	19991206 <--
EP 1137647	A1	20011004	EP 1999-965131	19991206 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
HU 2001004611	A2	20020429	HU 2001-4611	19991206 <--
HU 2001004611	A3	20021028		
JP 2002531557	T	20020924	JP 2000-586715	19991206 <--
ZA 2001004318	A	20020826	ZA 2001-4318	20010525 <--
NO 2001002837	A	20010719	NO 2001-2837	20010608 <--
MX 2001005835	A	20010911	MX 2001-5835	20010608 <--
PRIORITY APPLN. INFO.:			US 1998-207961	A 19981209 <--
			WO 1999-US28838	W 19991206 <--

OTHER SOURCE(S): MARPAT 133:30666

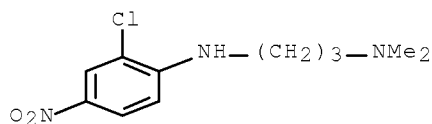
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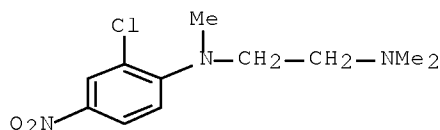
- AB Title compds. I and related compds. and their pharmaceutical salts are disclosed [wherein A = heteroaryl; R1-R4 = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, cyano; R1R2 or R3R4 = C5-7 aryl fusion; G = aryl or heteroaryl; and X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph or PhCH2; n = 1-6]. The compds. are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), and varicella-zoster virus (VZV), as well as (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 35 compds. in 2-4 bioassays. For instance, the pyridine derivative II had an IC50 of 0.018 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.
- IT 151951-35-8 338981-22-9 821776-85-6
821777-03-1 1098071-56-7
RL: PRPH (Prophetic)
(Aryl- and heteroaryl-substituted thiourea derivatives useful as inhibitors of herpes viruses)
- RN 151951-35-8 ZCAPLUS
- CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



- RN 338981-22-9 ZCAPLUS
- CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



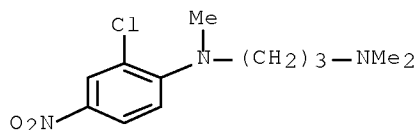
- RN 821776-85-6 ZCAPLUS
- CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)



10/560012

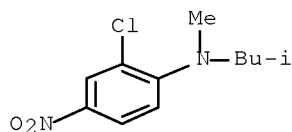
RN 821777-03-1 ZCAPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



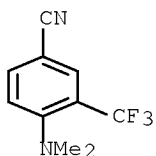
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of heteroaryl thiourea derivs. as inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 15 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401809 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:30657

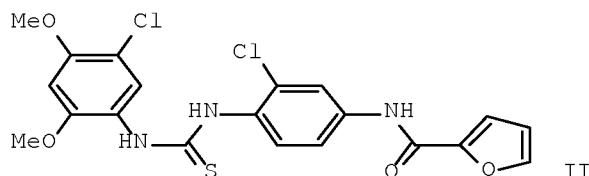
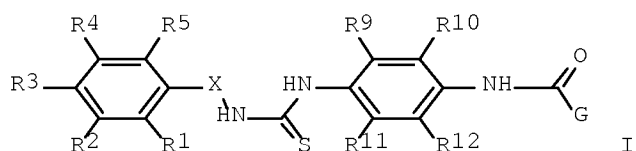
TITLE: Heterocyclic carboxamide-containing thiourea derivatives containing a substituted phenylenediamine group, useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi,

10/560012

Martin Joseph; Dushin, Russell George; Jones, Thomas
 Richard; Lang, Stanley Albert; Ross, Adma Antonia;
 Terefenko, Eugene Anthony; O'Hara, Bryan Mark
 PATENT ASSIGNEE(S): American Home Products Corporation, USA
 SOURCE: PCT Int. Appl., 159 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034261	A2	20000615	WO 1999-US28916	19991206 <--
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6166028	A	20001226	US 1999-444782	19991122 <--
US 6197803	B1	20010306	US 1999-447006	19991122 <--
US 6201013	B1	20010313	US 1999-444075	19991122 <--
CA 2351690	A1	20000615	CA 1999-2351690	19991206 <--
EP 1144399	A2	20011017	EP 1999-967213	19991206 <--
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JP 2002533301	T	20021008	JP 2000-586708	19991206 <--
HU 2002003405	A2	20030228	HU 2002-3405	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
US 6271236	B1	20010807	US 2000-669943	20000926 <--
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US 6555561	B2	20030429		
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			US 1998-155240P	P 19981209 <--
			US 1998-208540	A 19981209 <--
			US 1998-208561	A 19981209 <--
			US 1999-444782	A3 19991122 <--
			WO 1999-US28916	W 19991206 <--
			US 2000-669535	A3 20000926 <--
OTHER SOURCE(S):			MARPAT 133:30657	
GI				



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO₂, CO₂R₆, COR₆, OR₆, SR₆, SOR₆, SO₂R₆, CONR₇R₈, NR₆N(R₇R₈), N(R₇R₈), or W-Y-(CH₂)_n-Z, provided that at least 1 of R1-R5 ≠ H; or R₂R₃ or R₃R₄ form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R₆, R₇ = H, C1-6 alkyl or perhaloalkyl, or aryl; R₈ = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR₇R₈ forms 3- to 7-membered heterocycloalkyl; R₉-R₁₂ = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R₉R₁₀ or R₁₁R₁₂ = C5-7 aryl fusion, provided that at least 1 of R₉-R₁₂ ≠ H; W = O, NR₆, or bond; Y = CO, CO₂, or bond; Z = C1-4 alkyl, CN, CO₂R₆, COR₆, CONR₇R₈, OCOR₆, NR₆COR₇, OCONR₆, OR₆, SR₆, SOR₆, SO₂R₆, SR₆N(R₇R₈), N(R₇R₈) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)_J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH₂; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for 18 compds. in 4 bioassays. For instance, the N-(4-thioureidophenyl)furan-2-carboxamide derivative II had an IC₅₀ of 0.4 μg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.5 μg/mL against HSV in an ELISA assay.

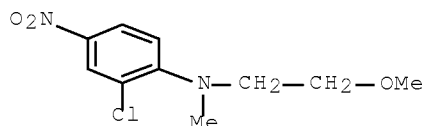
IT 151951-35-8 338981-22-9 821776-85-6
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Heterocyclic carboxamide-containing thiourea derivatives containing a substituted phenylenediamine group, useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

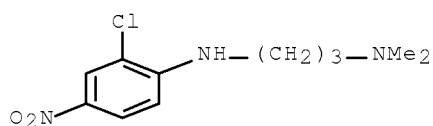
CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



10/560012

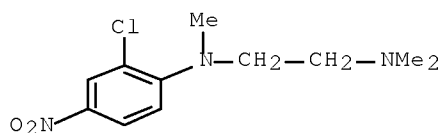
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CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



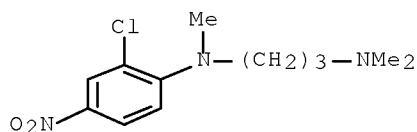
RN 821776-85-6 ZCAPLUS

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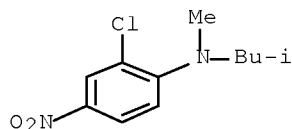
RN 821777-03-1 ZCAPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



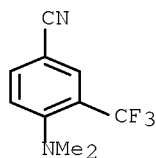
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of heterocyclic carboxamide-containing and phenylenediamine-containing thiourea derivs. as inhibitors of herpes

10/560012

viruses)
 RN 71145-96-5 ZCAPLUS
 CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 16 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401808 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:30588

TITLE: Alpha-methylbenzyl-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 168 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

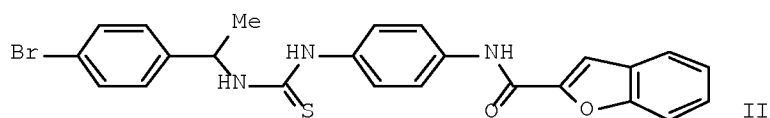
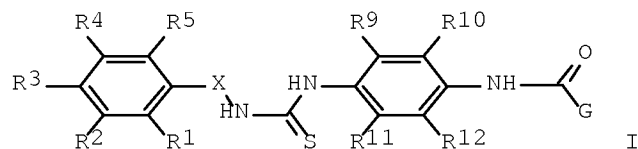
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034260	A2	20000615	WO 1999-US28839	19991206 <--
WO 2000034260	A3	20000908		
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1137645	A2	20011004	EP 1999-963022	19991206 <--
EP 1137645	B1	20040526		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
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HU 2001004492	A3	20021228		
JP 2002531555	T	20020924	JP 2000-586707	19991206 <--
NZ 512135	A	20031219	NZ 1999-512135	19991206 <--
AT 267824	T	20040615	AT 1999-963022	19991206 <--
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PT 1137645	T	20040930	PT 1999-963022	19991206 <--

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ES 2221470	T3	20041216	ES 1999-963022	19991206 <--
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PRIORITY APPLN. INFO.:			US 1998-208902	A 19981209 <--
			WO 1999-US28839	W 19991206 <--

OTHER SOURCE(S): MARPAT 133:30588

GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO₂, CO₂R₆, COR₆, OR₆, SR₆, SOR₆, SO₂R₆, CONR₇R₈, NR₆N(R₇R₈), N(R₇R₈), or W-Y-(CH₂)_n-Z, provided that at least 1 of R1-R5 ≠ H; or R₂R₃ or R₃R₄ form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R₆, R₇ = H, C1-6 alkyl or perhaloalkyl, or aryl; R₈ = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR₇R₈ forms 3- to 7-membered heterocycloalkyl; R₉-R₁₂ = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R₉R₁₀ or R₁₁R₁₂ = C5-7 aryl fusion; W = O, NR₆, or bond; Y = CO, CO₂, or bond; Z = C1-4 alkyl, CN, CO₂R₆, COR₆, CONR₇R₈, OCOR₆, NR₆COR₇, OCONR₆, OR₆, SR₆, SOR₆, SO₂R₆, SR₆N(R₇R₈), N(R₇R₈) or Ph; G = aryl or fused bicyclic aryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH₂; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 320 compds. in 1-4 bioassays. For instance, the [[(phenylethyl)thiourea]phenyl]benzofurancarboxamide derivative II had an IC₅₀ of 1.3 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.10 µg/mL against VZV in an ELISA assay.

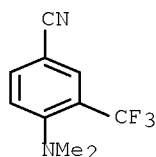
IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of α-methylbenzyl-containing thiourea derivs. as inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 17 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401806 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:30733

TITLE: Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Jones, Thomas Richard; Lang, Stanley Albert; Ross, Adma Antonia; Terefenko, Eugene Anthony; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 188 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

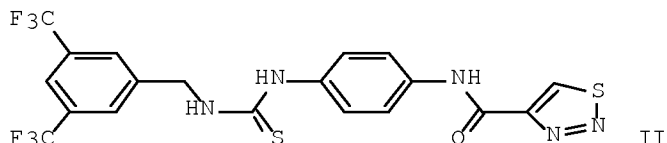
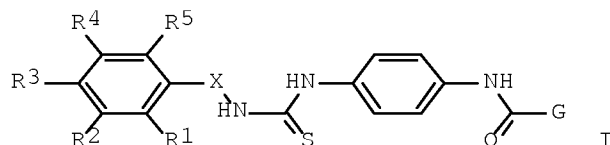
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034258	A2	20000615	WO 1999-US28842	19991206 <--
WO 2000034258	A3	20011129		
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RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6197803	B1	20010306	US 1999-447006	19991122 <--
CA 2350767	A1	20000615	CA 1999-2350767	19991206 <--
BR 9916046	A	20011002	BR 1999-16046	19991206 <--
EP 1144397	A2	20011017	EP 1999-963023	19991206 <--
EP 1144397	A3	20020911		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
TR 200101664	T2	20020321	TR 2001-1664	19991206 <--
HU 2002000232	A2	20020529	HU 2002-232	19991206 <--
JP 2002531554	T	20020924	JP 2000-586705	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
US 6271236	B1	20010807	US 2000-669943	20000926 <--
ZA 2001004377	A	20021220	ZA 2001-4377	20010528 <--
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NO 2001002832	A	20010807	NO 2001-2832	20010608 <--
BG 105581	A	20011231	BG 2001-105581	20010608 <--
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US 6555561	B2	20030429		

10/560012

PRIORITY APPLN. INFO.:

US 1998-208559	A	19981209	<--
US 1998-150692P	P	19981209	<--
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WO 1999-US28842	W	19991206	<--
US 2000-669535	A3	20000926	<--

OTHER SOURCE(S): MARPAT 133:30733
GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO2, CO2R6, COR6, OR6, SR6, SOR6, SO2R6, CONR7R8, NR6N(R7R8), N(R7R8), or W-Y-(CH2)n-Z, provided that at least 1 of R1-R5 ≠ H; or R2R3 or R3R4 form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R6, R7 = H, C1-6 alkyl or perhaloalkyl, or aryl; R8 = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR7R8 forms 3- to 7-membered heterocycloalkyl; W = O, NR6, or bond; Y = CO, CO2, or bond; Z = C1-4 alkyl, CN, CO2R6, COR6, CONR7R8, OCOR6, NR6COR7, OCONR6, OR6, SR6, SOR6, SO2R6, SR6N(R7R8), N(R7R8) or Ph; G = monocyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH2; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 350 compds. in 1-4 bioassays. For instance, the thioureidophenylthiadiazolecarboxamide derivative II had an IC50 of 0.0011 µg/mL against HCMV wild-type in human foreskin fibroblast cell culture.

IT 151951-35-8 338981-22-9 821776-85-6
821777-03-1 1098071-56-7

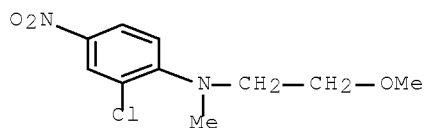
RL: PRPH (Prophetic)

(Heterocyclic carboxamide-containing thiourea derivatives containing a phenylenediamine group, useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

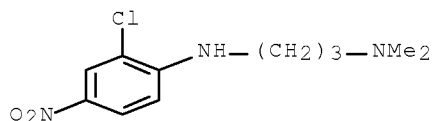
CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)

10/560012



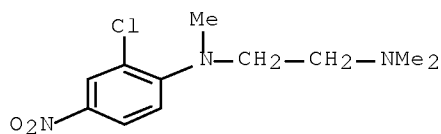
RN 338981-22-9 ZCAPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



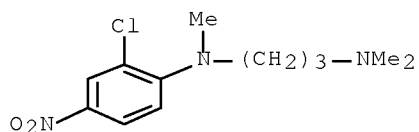
RN 821776-85-6 ZCAPLUS

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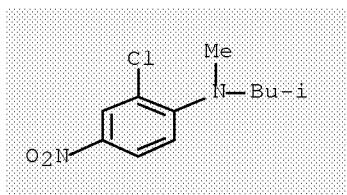
CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

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10/560012



IT 71145-96-5

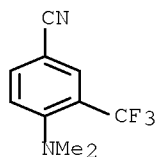
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of heterocyclic carboxamide-containing thiourea

derivs. as inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 18 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401786 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 133:30587

TITLE: Benzamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Curran, Kevin Joseph; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; Norton, Emily Boucher; Ross, Adma Antonia; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000034238	A1	20000615	WO 1999-US28837	19991206 <--
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US 6207715	B1	20010327	US 1999-444897	19991122 <--
US 6255349	B1	20010703	US 1999-444734	19991122 <--
US 6262090	B1	20010717	US 1999-444896	19991122 <--
US 6335350	B1	20020101	US 1999-447005	19991122 <--
CA 2351403	A1	20000615	CA 1999-2351403	19991206 <--
BR 9916086	A	20010904	BR 1999-16086	19991206 <--
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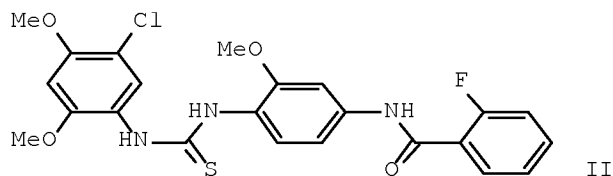
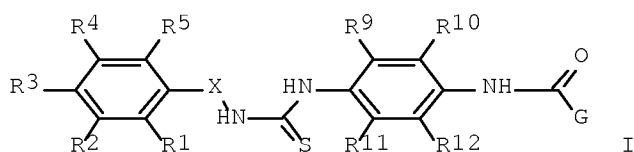
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

TR 200101597	T2	20011022	TR 2001-1597	19991206 <--
HU 2001004763	A2	20020429	HU 2001-4763	19991206 <--
HU 2001004763	A3	20050428		
JP 2002531545	T	20020924	JP 2000-586686	19991206 <--
NZ 512108	A	20030926	NZ 1999-512108	19991206 <--
AT 272052	T	20040815	AT 1999-963021	19991206 <--
PT 1137632	T	20041130	PT 1999-963021	19991206 <--
ES 2224733	T3	20050301	ES 1999-963021	19991206 <--
US 6262082	B1	20010717	US 2000-669483	20000925 <--
US 6271236	B1	20010807	US 2000-669943	20000926 <--
US 6403617	B1	20020611	US 2000-669535	20000926 <--
US 6407123	B1	20020618	US 2000-670180	20000926 <--
US 6426355	B1	20020730	US 2000-671486	20000927 <--
US 6407249	B1	20020618	US 2000-684011	20001229 <--
US 6410571	B1	20020625	US 2000-684773	20001229 <--
US 20020026055	A1	20020228	US 2001-804510	20010312 <--
US 6380243	B2	20020430		
US 20010039348	A1	20011108	US 2001-845428	20010430 <--
US 6462055	B2	20021008		
ZA 2001004144	A	20020821	ZA 2001-4144	20010521 <--
NO 2001002838	A	20010808	NO 2001-2838	20010608 <--
MX 2001005829	A	20010911	MX 2001-5829	20010608 <--
BG 105583	A	20011231	BG 2001-105583	20010608 <--
US 20030036653	A1	20030220	US 2002-99695	20020315 <--
US 6555561	B2	20030429		

PRIORITY APPLN. INFO.:

US 1998-208561	A	19981209 <--
US 1998-228805P	P	19981209 <--
US 1998-228808P	P	19981209 <--
US 1998-228809P	P	19981209 <--
US 1998-150692P	P	19981209 <--
US 1998-150698P	P	19981209 <--
US 1998-155192P	P	19981209 <--
US 1998-155240P	P	19981209 <--
US 1998-208164	A	19981209 <--
US 1998-208540	A	19981209 <--
US 1999-444734	A3	19991122 <--
US 1999-444782	A3	19991122 <--
US 1999-444896	A3	19991122 <--
US 1999-447006	A3	19991122 <--
WO 1999-US28837	W	19991206 <--
US 2000-669535	A3	20000926 <--

OTHER SOURCE(S): MARPAT 133:30587
GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO₂, CO₂R₆, COR₆, OR₆, SR₆, SOR₆, SO₂R₆, CONR₇R₈, NR₆N(R₇R₈), N(R₇R₈), or W-Y-(CH₂)_n-Z, provided that at least 1 of R1-R5 ≠ H; or R₂R₃ or R₃R₄ form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R₆, R₇ = H, C1-6 alkyl or perhaloalkyl, or aryl; R₈ = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR₇R₈ forms 3- to 7-membered heterocycloalkyl; R₉-R₁₂ = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R₉R₁₀ or R₁₁R₁₂ = C5-7 aryl fusion, provided that at least 1 of R₉-R₁₂ ≠ H; W = O, NR₆, or bond; Y = CO, CO₂, or bond; Z = C1-4 alkyl, CN, CO₂R₆, COR₆, CONR₇R₈, OCOR₆, NR₆COR₇, OCONR₆, OR₆, SR₆, SOR₆, SO₂R₆, SR₆N(R₇R₈), N(R₇R₈) or Ph; G = aryl or fused bicyclic heteroaryl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH₂; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 75 compds. in 2-4 bioassays. For instance, the thioureidophenylbenzamide derivative II had an IC₅₀ of 1.5 μg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 0.04 μg/mL against HSV in an ELISA assay.

IT 151951-35-8 338981-22-9 821776-85-6

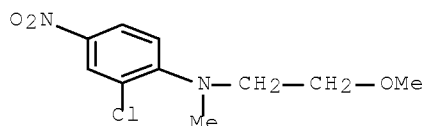
821777-03-1 1098071-56-7

RL: PRPH (Prophetic)

(Benzamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

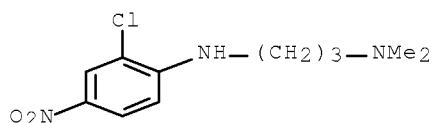
CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



10/560012

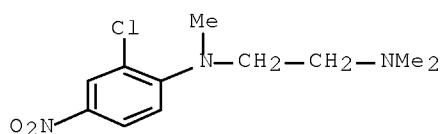
RN 338981-22-9 ZCAPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



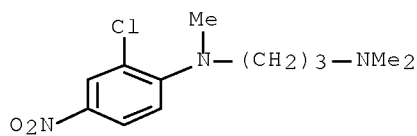
RN 821776-85-6 ZCAPLUS

CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)



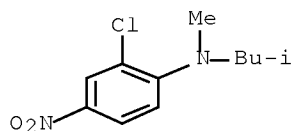
RN 821777-03-1 ZCAPLUS

CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)



IT 71145-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of benzamide-containing aryl thiourea

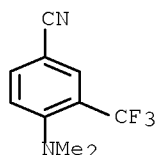
10/560012

derivs. as

inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 19 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:401785 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:30586

TITLE: Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses

INVENTOR(S): Bloom, Jonathan David; Digrandi, Martin Joseph; Dushin, Russell George; Lang, Stanley Albert; O'Hara, Bryan Mark

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE: ~~Patent~~

LANGUAGE: English

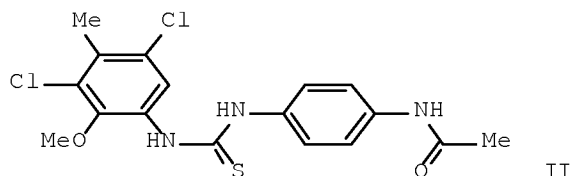
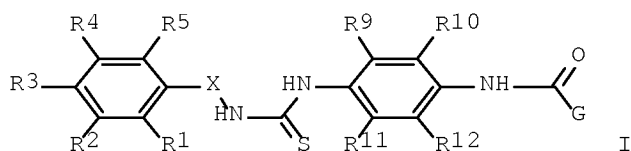
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034237	A2	20000615	WO 1999-US28844	19991206 <--
WO 2000034237	A3	20001123		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2350899	A1	20000615	CA 1999-2350899	19991206 <--
EP 1137633	A2	20011004	EP 1999-965132	19991206 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9916041	A	20011204	BR 1999-16041	19991206 <--
HU 2001004944	A2	20020429	HU 2001-4944	19991206 <--
HU 2001004944	A3	20030328		
JP 2002531544	T	20020924	JP 2000-586685	19991206 <--
ZA 2001004142	A	20021025	ZA 2001-4142	20010521 <--
MX 2001005680	A	20010911	MX 2001-5680	20010606 <--
NO 2001002834	A	20010807	NO 2001-2834	20010608 <--
PRIORITY APPLN. INFO.:			US 1998-208316	A 19981209 <--
			WO 1999-US28844	W 19991206 <--

10/560012

OTHER SOURCE(S): MARPAT 133:30586
GI



AB Title compds. I and related compds. are disclosed [wherein R1-R5 = H, C1-6 alkyl or perhaloalkyl, C2-6 alkenyl or alkynyl, C3-10 (hetero)cycloalkyl, (hetero)aryl, halo, CN, NO₂, CO₂R₆, COR₆, OR₆, SR₆, SOR₆, SO₂R₆, CONR₇R₈, NR₆N(R₇R₈), N(R₇R₈), or W-Y-(CH₂)_n-Z, provided that at least 1 of R1-R5 ≠ H; or R₂R₃ or R₃R₄ form 3- to 7-membered heterocycloalkyl or heteroaryl fusion; R₆, R₇ = H, C1-6 alkyl or perhaloalkyl, or aryl; R₈ = H, C1-6 alkyl or perhaloalkyl, C3-10 (hetero)cycloalkyl, (hetero)aryl; or NR₇R₈ forms 3- to 7-membered heterocycloalkyl; R₉-R₁₂ = H, C1-4 alkyl or perhaloalkyl, halo, C1-4 alkoxy, or cyano, or R₉R₁₀ or R₁₁R₁₂ = C5-7 aryl fusion; W = O, NR₆, or bond; Y = CO, CO₂, or bond; Z = C1-4 alkyl, CN, CO₂R₆, COR₆, CONR₇R₈, OCOR₆, NR₆COR₇, OCONR₆, OR₆, SR₆, SOR₆, SO₂R₆, SR₆N(R₇R₈), N(R₇R₈) or Ph; G = C1-6 alkyl; X = bond, NH, C1-6 alkyl, alkenyl, alkoxy, alkylthio, or alkylamino, or (CH)J; J = C1-6 alkyl, C3-7 cycloalkyl, Ph, or PhCH₂; n = 1-6]. I, or pharmaceutical salts thereof, are useful in the treatment of diseases associated with herpes viruses, including human cytomegalovirus (HCMV), herpes simplex viruses (HSV), varicella-zoster virus (VZV), or (no data) Epstein-Barr virus, human herpesviruses-6 and -7, and Kaposi herpesvirus. Approx. 1000 example compds. prepared by standard methods are listed, with biol. data for approx. 160 compds. in 4 bioassays. For instance, the thioureidophenylacetamide derivative II had an IC₅₀ of 0.8 μg/mL against HCMV wild-type in human foreskin fibroblast cell culture, and 2 μg/mL against HSV in an ELISA assay.

IT 151951-35-8 338981-22-9 821776-85-6
821777-03-1 1098071-56-7

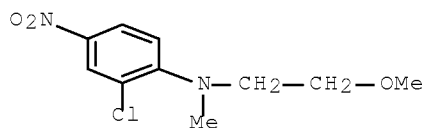
RL: PRPH (Prophetic)

(Acetamide and substituted acetamide-containing aryl thiourea derivatives useful as inhibitors of herpes viruses)

RN 151951-35-8 ZCAPLUS

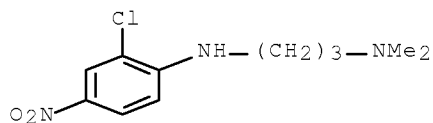
CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)

10/560012



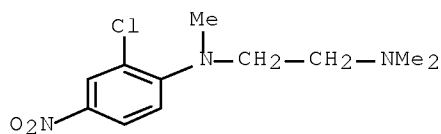
RN 338981-22-9 ZCAPLUS

CN 1,3-Propanediamine, N3-(2-chloro-4-nitrophenyl)-N1,N1-dimethyl- (CA INDEX NAME)



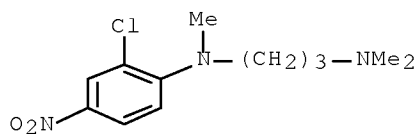
RN 821776-85-6 ZCAPLUS

CN 1,2-Ethanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N2,N2-trimethyl- (CA INDEX NAME)



RN 821777-03-1 ZCAPLUS

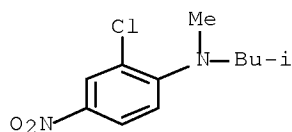
CN 1,3-Propanediamine, N1-(2-chloro-4-nitrophenyl)-N1,N3,N3-trimethyl- (CA INDEX NAME)



RN 1098071-56-7 ZCAPLUS

CN Benzenamine, 2-chloro-N-methyl-N-(2-methylpropyl)-4-nitro- (CA INDEX NAME)

10/560012



IT 71145-96-5

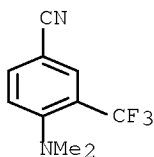
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of acetamide-containing aryl thiourea
derivs. as

inhibitors of herpes viruses)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 20 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:259962 ZCAPLUS Full-text

DOCUMENT NUMBER: 132:283910

TITLE: Agent and method for dyeing fibers

INVENTOR(S): Braun, Hans-Juergen; Semadeni, Pascal Andre

PATENT ASSIGNEE(S): Wella Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DOCUMENT TYPE: ~~Patent~~

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2000021496	A1	20000420	WO 1999-EP6601	19990908 <--
W: BR, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19847192	A1	20000427	DE 1998-19847192	19981013 <--
EP 1037593	A1	20000927	EP 1999-944624	19990908 <--
EP 1037593	B1	20040204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9906871	A	20001017	BR 1999-6871	19990908 <--
JP 2002527369	T	20020827	JP 2000-575472	19990908 <--
AT 258782	T	20040215	AT 1999-944624	19990908 <--
ES 2214882	T3	20040916	ES 1999-944624	19990908 <--
US 6379400	B1	20020430	US 2000-581367	20000612 <--

10/560012

PRIORITY APPLN. INFO.:

DE 1998-19847192

A 19981013 <--

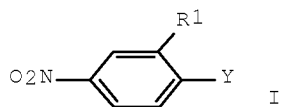
WO 1999-EP6601

W 19990908 <--

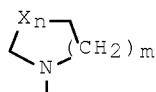
OTHER SOURCE(S):

MARPAT 132:283910

GI



I



II

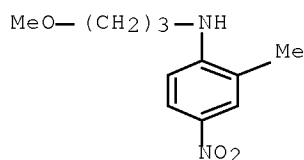
AB Direct dyes for fibers, especially hair, which contain 4-nitrophenylamine derivs. I [R1 = H, C1-4 alkyl; Y = II, cycloalkyl, NR2R3, (CH2)zOR4; ≥1 of R2, R3 ≠ H; R4 = C1-4 alkyl; X = N, O; m = 1-3; n = 0, 1; z = 1-6] are prepared which are readily water soluble, fast towards light, friction, permanent waving, and perspiration, and produce a brilliant yellow coloration. I can be used in conjunction with other direct dyes or with oxidative dyes. Thus, 1-fluoro-4-nitrobenzene reacted with 1-amino-2-methoxyethane to form N-(2-methoxyethyl)-4-nitrophenylamine (III). A composition containing III 0.49, iso-PrOH 10.00, 28% aqueous lauryl alc. diglycol ether sulfate Na salt 10.00, and H2O to 100.00 g was adjusted to pH 5 or 8 and applied to bleached hair at 40° for 40 min to produce an intense lemon-yellow color at either pH.

IT 263902-65-4P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(agent and method for dyeing fibers)

RN 263902-65-4 ZCAPLUS

CN Benzenamine, N-(3-methoxypropyl)-2-methyl-4-nitro- (CA INDEX NAME)



REFERENCE COUNT:

8

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 21 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:125899 ZCAPLUS Full-text

DOCUMENT NUMBER: 128:250295

ORIGINAL REFERENCE NO.: 128:49441a, 49444a

TITLE: Pattern recognition corresponding analysis of powder frequency doubling effect of the nitrobenzene derivatives

AUTHOR(S): Yang, Rongsheng; Chen, Jiangzhong; Zhang, Hanhui

CORPORATE SOURCE: Department of Chemistry, Fuzhou University, Fuzhou, 350002, Peop. Rep. China

SOURCE: Fuzhou Daxue Xuebao, Ziran Kexueban (1997), 25(3), 95-98

CODEN: FDXKEN; ISSN: 1000-2243

10/560012

PUBLISHER: Fuzhou Daxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The relationship between the structure and powder frequency doubling effect was studied by pattern recognition corresponding anal. method to avoid space group problems. Two groups of binding relationships were formulated, which can predict crystals with higher powder frequency doubling effect. Path for mol. engineering and crystal engineering was discussed.

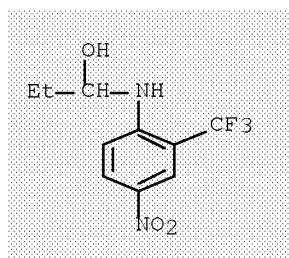
IT 204931-24-8

RL: PRP (Properties)

(pattern recognition corresponding anal. of powder frequency doubling effect of nitrobenzene derivative)

RN 204931-24-8 ZCAPLUS

CN 1-Propanol, 1-[[4-nitro-2-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



L70 ANSWER 22 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:89624 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 128:192539

ORIGINAL REFERENCE NO.: 128:38035a,38038a

TITLE: The reactivity of nitrophenyl-substituted cyclic amines in dehydrogenations

AUTHOR(S): Moehrle, H.; Mehrens, J.

CORPORATE SOURCE: Institut Pharmazeutische Chemie,
Heinrich-Heine-Universitaet, Duesseldorf, D-40225,
Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences
(1998), 53(1), 37-48

CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 128:192539

AB 1-(4-Nitrophenyl)-substituted piperidine and perhydroazepine were inert to Hg(II)-EDTA, while the corresponding α -pipecoline gave an amino ketone with ring cleavage. However, the corresponding 2-nitrophenyl compds. reacted to give a 2-piperidinone, an aminopentanal, and an aminohexanone, resp. By an addnl. substituent in 2'-position the 4-nitro compds. underwent dehydrogenation too. With a Me group resulted a pattern analogous to 2-nitro products. A neighboring CH₂OH function enhanced the reaction with formation of benzoxazines and if possible their further oxidized derivs., hydroxy lactams.

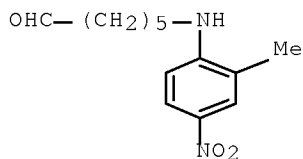
IT 203510-10-5F

RL: SPN (Synthetic preparation); PREP (Preparation)

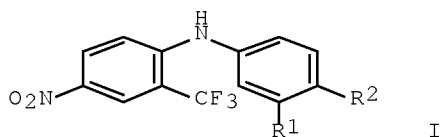
(dehydrogenation of nitrophenyl-substituted cyclic amines)

RN 203510-10-5 ZCAPLUS

CN Hexanal, 6-[(2-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



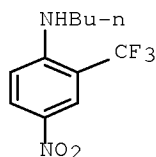
L70 ANSWER 23 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:561104 ZCAPLUS Full-text
 DOCUMENT NUMBER: 125:275309
 ORIGINAL REFERENCE NO.: 125:51485a,51488a
 TITLE: Synthesis of substituted diphenylamines under phase transfer catalysis
 AUTHOR(S): Durantini, Edgardo N.; Chiacchiera, Stella M.; Silber, Juana J.
 CORPORATE SOURCE: Dep. Quim. Fis., Univ. Nacl. Rio Cuarto, Rio Cuarto, 5800, Argent.
 SOURCE: Synthetic Communications (1996), 26(20), 3849-3858
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Dekker
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:275309
 GI



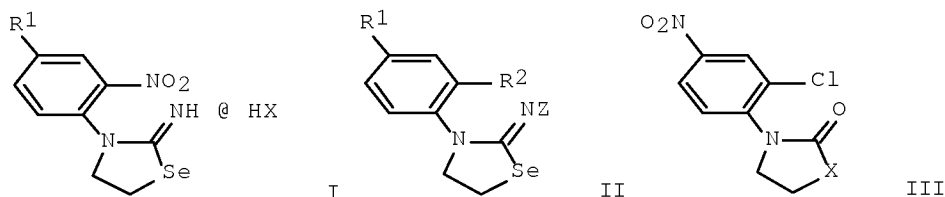
AB A convenient procedure for the synthesis of N-[(trifluoromethyl)nitrophenyl] substituted anilines, e.g., I (R1 = H, R2 = NO2; R1 = NO2, R2 = H; R1 = H, R2 = cyano), by means of a chloro-substitution reaction under conditions of phase-transfer catalysis (PTC) is reported. The ipso-substitution product is obtained with high yield. This method provides a general procedure for the synthesis of diphenylamines bearing electron-withdrawing groups in both aromatic rings.

IT 175873-18-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of diphenylamines under phase transfer catalysis)

RN 175873-18-4 ZCAPLUS
 CN Benzenamine, N-butyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



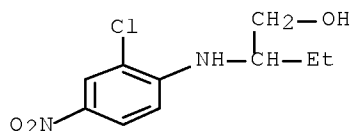
L70 ANSWER 24 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:426976 ZCAPLUS Full-text
 DOCUMENT NUMBER: 125:195846
 ORIGINAL REFERENCE NO.: 125:36687a,36690a
 TITLE: Synthesis, some reactions and anti-ulcer activity of
 some 2-amino-3-(substituted phenyl)selenazolidines
 AUTHOR(S): Hornyak, Gyula; Feller, Antal; Lempert, Karoly
 CORPORATE SOURCE: Res. Group Alkaloid Chem., Hungarian Academy Sci.,
 Budapest, H-1521, Hung.
 SOURCE: ACH - Models in Chemistry (1995), 132(6), 871-885
 CODEN: ACMCEI; ISSN: 1217-8969
 PUBLISHER: Akademiai Kiado
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:195846
 GI



AB 2-Imino-3-(substituted phenyl)selenazolidine salts, e.g., I (R1 = H, NO2, CF3, X = Cl, Br), were prepared (1) by acid induced ring closure of N-(2-selenocyanatoethyl)anilines, or (2) by fusion of anilines with 2-bromoethylselenocyanate. E.g., 2-NO2C6H4NHCH2CH2SeCN is refluxed in dioxane the presence of ethanesulfonic acid to give I (R1 = H, HX = HO3SEt) in 93% yield. Diselenide, e.g., (ArNHCH2CH2Se)2, formation accompanying the syntheses according to Method 1 above was successfully suppressed. Some N-substituted derivs. (e.g., II, R1 ≠ R2 = Cl, NO2, Z = CHO, Ac, CONHPr, SO2Et) of selenazolidines I, as well as 3-aryl-selenazolidin-2-one III (X = Se), and its thiazolidinone analog III (X = S), were also prepared. The gastroprotective (antiulcer) activity of some of I, II and III is reported.

IT 180691-77-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and methylsulfonylation in the synthesis of amino(substituted phenyl)selenazolidines as antiulcer agents)

RN 180691-77-4 ZCAPLUS
 CN 1-Butanol, 2-[(2-chloro-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 25 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:259463 ZCAPLUS Full-text
 DOCUMENT NUMBER: 124:288977
 ORIGINAL REFERENCE NO.: 124:53579a,53582a
 TITLE: Preparation of nitroarylamines
 INVENTOR(S): Jautelat, Manfred
 PATENT ASSIGNEE(S): Bayer A.-G., Germany
 SOURCE: Eur. Pat. Appl., 7 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 695737	A1	19960207	EP 1995-111426	19950720 <--
EP 695737	B1	19970618		
R: BE, DE, FR, GB, IT, NL				
DE 4427249	A1	19960208	DE 1994-4427249	19940802 <--
US 5684203	A	19971104	US 1995-504034	19950726 <--
CA 2154965	A1	19960203	CA 1995-2154965	19950728 <--
JP 08059571	A	19960305	JP 1995-211399	19950728 <--
PRIORITY APPLN. INFO.:			DE 1994-4427249	A 19940802 <--

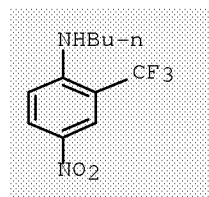
OTHER SOURCE(S): CASREACT 124:288977; MARPAT 124:288977

AB RNHZ(X_n)NO₂ [R = H, (cyclo)alkyl, alkenyl, aryl, etc.; X = halo, cyano, alkyl, alkoxy, etc.; Z = (n+2)-valent (hetero)aryl group; n = 0-3] were prepared by amination of Z(X_n)NO₂ [Z = (n+1)-valent (hetero)aryl group] by (RNH)₂CY (Y = O or S) in the presence of a base, O, and a dipolar solvent. Thus, 3-(F₃C)C₆H₄NO₂ was heated 4h at 50° with (MeNH)₂CO in DMSO containing NaOH and with air sparging to give 100% N-methyl-4-nitro-2-trifluoromethylaniline.

IT 175873-18-4P, N-Butyl-4-nitro-2-trifluoromethylaniline
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of nitroarylamines)

RN 175873-18-4 ZCAPLUS

CN Benzenamine, N-butyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)

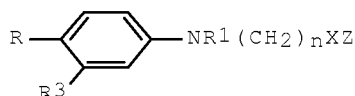


L70 ANSWER 26 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:169712 ZCAPLUS Full-text
 DOCUMENT NUMBER: 122:31106
 ORIGINAL REFERENCE NO.: 122:6139a,6142a
 TITLE: Preparation of p-phenylenediamines
 INVENTOR(S): Urano, Fumyoshi; Kimura, Takahiro; Kametani, Miki
 PATENT ASSIGNEE(S): Wako Pure Chem Ind Ltd, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: ~~Patent~~
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06219997	A	19940809	JP 1993-28593	19930125 <--
PRIORITY APPLN. INFO.:			JP 1993-28593	19930125 <--
OTHER SOURCE(S):		CASREACT 122:31106; MARPAT 122:31106		

GI



I

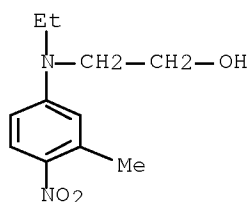
AB The title compds. [I; R = NH2; R1 = C1-3 alkyl; R3 = H, C1-3 alkyl, C1-3 alkoxy; X = O, NH; Z = H, COR4, SO2R4; R4 = C1-3 alkyl, (alkyl)phenyl; n = 1-3], useful as intermediates for azo dyes, pharmaceuticals, and agrochems. and photog. developers (no data), are prepared by nitration of I [R = H; Z = YR2; R2 = C1-3 alkyl, (alkyl)phenyl; Y = CO, SO2], treatment with H2O or alkaline aqueous solns., and reduction of the resulting I (R = NO2; Z = H, COR4, SO2R4). I (R = H, R1 = Et, R3 = Me, XZ = OAc, n = 2) (preparation given) was nitrated by HNO3 and H2SO4 at -5 to 0° for 3 h and treated with aqueous NaOH in MeOH at 25-30° for 2 h to give 99% I (R = NO2, R1 = Et, R3 = Me, XZ = OH, n = 2), which was reduced by H with Pd/C in EtOH at 25-35° for 6 h to give 95% sulfate salt of I (R = NH2, R1 = Et, R3 = Me, XZ = OH, n = 2).

IT 52177-13-6P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of phenylenediamines from anilines via nitroanilines)

RN 52177-13-6 ZCAPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 27 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:77020 ZCAPLUS Full-text

DOCUMENT NUMBER: 120:77020

ORIGINAL REFERENCE NO.: 120:13849a,13852a

TITLE: Preparation of N-alkoxyalkyl p-phenylenediamine
developers for oxidative hair dyes

INVENTOR(S): Rose, David; Lieske, Edgar; Hoeffkes, Horst

PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany

SOURCE: Ger. Offen., 7 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

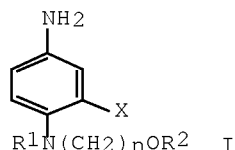
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4205329	A1	19930826	DE 1992-4205329	19920221 <--
WO 9316679	A1	19930902	WO 1993-EP351	19930213 <--

W: JP, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRIORITY APPLN. INFO.: DE 1992-4205329 A 19920221 <--

OTHER SOURCE(S): MARPAT 120:77020

GI



AB Title compds. (I; R1, R2 = alkyl; X = H, halo; n = 2-4), were prepared Thus, 4-FC6H4NO2, CaCO3, and MeNHCH2CH2OMe were refluxed in acetone to give 4-O2NC6H4NMeCH2CH2OMe, which was hydrogenated followed by salification with HCl to give 4-H2NC6H4NMeCH2CH2OMe.2HCl. This developer together with 2-chloro-3-amino-6methylphenol coupler and 3% H2O3 oxidizer gave a blue-black color to gray hair.

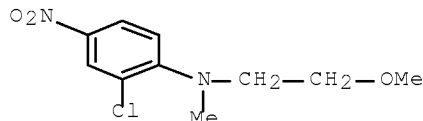
IT 151951-35-8F

RL: PREP (Preparation)

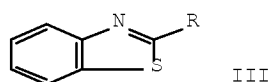
(prepare of, as intermediate for developer for oxidative hair dyes)

RN 151951-35-8 ZCAPLUS

CN Benzenamine, 2-chloro-N-(2-methoxyethyl)-N-methyl-4-nitro- (CA INDEX NAME)



L70 ANSWER 28 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1991:247193 ZCAPLUS Full-text
 DOCUMENT NUMBER: 114:247193
 ORIGINAL REFERENCE NO.: 114:41737a,41740a
 TITLE: Acyclic tertiary amines as nucleophiles in substitution reactions of aromatic and heteroaromatic halides
 AUTHOR(S): Matsumoto, Kiyoshi; Hashimoto, Shiro; Otani, Shinichi
 CORPORATE SOURCE: Coll. Lib. Arts Sci., Kyoto Univ., Kyoto, 606, Japan
 SOURCE: Journal of the Chemical Society, Chemical Communications (1991), (5), 306-7
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



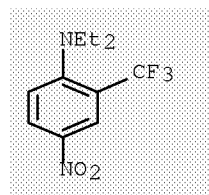
AB Even acyclic tertiary amines such as Et₃N, Pr₃N and Bu₃N, which have been believed to be inert to aromatic and heteroarom. halides, underwent S_NAr reactions with aromatic and heteroarom. halides to give the dialkylamino derivs. via an addition-elimination mechanism; in the case of monocyclic amines like N-methylpyrrolidine (I) and N-methylpiperidine (II) the dealkylation being regioselective. Thus, the reaction of 2-chlorobenzothiazole III (R = Cl) with I and II gave 92-96% III (R = pyrrolidino, piperidino) resp.

IT 25900-35-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 25900-35-0 ZCAPLUS

CN Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)

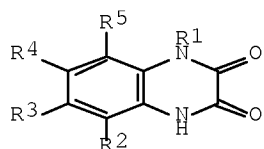


L70 ANSWER 29 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1989:632859 ZCAPLUS Full-text
 DOCUMENT NUMBER: 111:232859

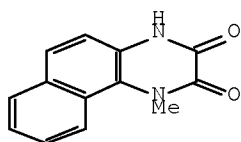
10/560012

ORIGINAL REFERENCE NO.: 111:38689a,38692a
 TITLE: Preparation and testing of
 2,3(1H,4H)-quinoxalinediones as neuroleptics
 INVENTOR(S): Honore, Tage; Jacobsen, Poul; Elmelund, Flemming;
 Naerum, Lars
 PATENT ASSIGNEE(S): Aktieselskabet Ferrosan, Den.
 SOURCE: Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 315959	A2	19890517	EP 1988-118592	19881108 <--
EP 315959	A3	19891227		
EP 315959	B1	19940302		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 164317	C	19921102	DK 1987-5862	19871110 <--
NO 8804729	A	19890511	NO 1988-4729	19881024 <--
NO 179551	B	19960722		
NO 179551	C	19961030		
CA 1321587	C	19930824	CA 1988-582104	19881103 <--
DK 8806206	A	19890511	DK 1988-6206	19881108 <--
DK 164317	B	19920609		
ZA 8808367	A	19890830	ZA 1988-8367	19881108 <--
US 4948794	A	19900814	US 1988-268939	19881108 <--
AT 102192	T	19940315	AT 1988-118592	19881108 <--
ES 2061606	T3	19941216	ES 1988-118592	19881108 <--
AU 8824949	A	19890511	AU 1988-24949	19881109 <--
AU 618766	B2	19920109		
FI 8805151	A	19890511	FI 1988-5151	19881109 <--
FI 100181	B1	19971015		
JP 01153680	A	19890615	JP 1988-282621	19881110 <--
JP 2721520	B2	19980304		
KR 9711279	B1	19970709	KR 1988-14744	19881110 <--
US 5026704	A	19910625	US 1989-456325	19891226 <--
NO 9603412	A	19890511	NO 1996-3412	19960815 <--
NO 307252	B1	20000306		
PRIORITY APPLN. INFO.:			DK 1987-5862	A 19871110 <--
			DK 1988-1422	A 19880316 <--
			NO 1988-4729	A 19881024 <--
			EP 1988-118592	A 19881108 <--
			US 1988-268939	A1 19881108 <--
OTHER SOURCE(S):			MARPAT 111:232859	
GI				



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II

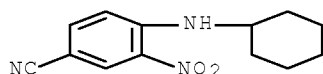
10/560012

AB The title compds. [I; R1 = C3-8 cycloalkyl, aryl, aralkyl, (un)substituted C1-12 alkyl; R2-R5 = H, CF3 C1-4 alkoxy, cyano, halo, NO2; R2R3, R4R5 = atoms to complete an (un)substituted, fused aromatic ring; when R1 = Me, R3 ≠ CF3, MeO, Br, Cl, NO2] were prepared as neurotransmitter antagonists, especially at NMDA (N-methyl-D-aspartate), quisqualate, and kainate receptors. I are useful as tranquilizers. 2-Bromo-6-methoxynaphthalene was nitrated to give 73% 6-bromo-2-methoxy-1-nitronaphthalene which was treated with MeNH2 in DMF to give 96% 6-bromo-N-methyl-1-nitro-2-naphthylamine. The latter was hydrogenated over Pd-C and the product was refluxed with (CO2H)2.2H2O in 4 M HCl to give 92% benzoquinoxalinedione II. II inhibited AMPA (α -amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid) binding to quisqualate receptors in rat cerebral cortical membrane preps. with an IC50 of 0.42 μ g/mL.

IT ~~28096-55-1F~~
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of tranquilizers)

RN 28096-55-1 ZCAPLUS

CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)



L70 ANSWER 30 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:486773 ZCAPLUS Full-text

DOCUMENT NUMBER: 111:86773

ORIGINAL REFERENCE NO.: 111:14447a,14450a

TITLE: Organic crystals for nonlinear optics: molecular engineering of non-centrosymmetric crystal structures

AUTHOR(S): Nicoud, J. F.

CORPORATE SOURCE: Inst. Phys. Chim. Mater., Inst. Charles Sadron, Strasbourg, F-67083, Fr.

SOURCE: Special Publication - Royal Society of Chemistry (1989), 69(Org. Mater. Non-linear Opt.), 157-62
CODEN: SROCDQ; ISSN: 0260-6291

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some recent results are presented concerning the use of chirality as an efficient strategy for the tentative control of non-centrosymmetry in organic crystals. In addition to the classical nitro-Ph or nitro-pyridine derivs., some new conjugated chains were studied, such as chalcone and 2-benzylidene-1,3-indanedione derivs. The nonlinear optical properties of these new materials were tested by 2nd-harmonic generation on crystalline powders, at 1.06 or 1.32 μ m.

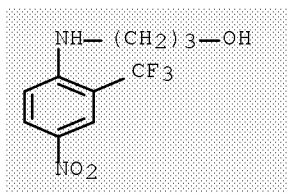
IT ~~115416-49-4~~ ~~115416-50-7~~

RL: PROC (Process)
(second-harmonic generation of)

RN 115416-49-4 ZCAPLUS

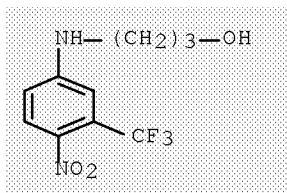
CN 1-Propanol, 3-[[4-nitro-2-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

10/560012



RN 115416-50-7 ZCAPLUS

CN 1-Propanol, 3-[[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



L70 ANSWER 31 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1988:463796 ZCAPLUS Full-text

DOCUMENT NUMBER: 109:63796

ORIGINAL REFERENCE NO.: 109:10551a,10554a

TITLE: Molecular and crystal engineering for organic nonlinear optical materials

AUTHOR(S): Nicoud, J. F.

CORPORATE SOURCE: ESPCI, UA, CNRS, Paris, 75231, Fr.

SOURCE: Molecular Crystals and Liquid Crystals (1988), 156(Pt. A), 257-68

CODEN: MCLCA5; ISSN: 0026-8941

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Nonlinear optical crystals are attractive due to their potential applications in optical signal processing. Several strategies were investigated to get efficient organic nonlinear optical crystals having enhanced quadratic responses and high efficiencies for 2nd harmonic generation. One chooses mols. with high mol. hyperpolarizability, β . Typical mols. possess a highly delocalized π -electron system bearing a donor and an acceptor group in such positions that an intramol. charge transfer occurs. These mols. must be assembled in an optimized acentric fashion to get a material having a high 2nd order elec. susceptibility, $\chi(2)$. The use of chirality to ensure noncentrosym. crystal structures, extra polar groups to influence dipole-dipole interactions, push-pull N-oxide bonds and H bonding were satisfactory strategies to get some of the most efficient organic crystals for nonlinear optics.

IT 115416-49-4P 115416-50-7P

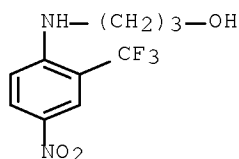
RL: PREP (Preparation)

(preparation of, in mol. and crystal engineering for organic nonlinear optical materials)

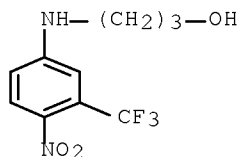
RN 115416-49-4 ZCAPLUS

CN 1-Propanol, 3-[[4-nitro-2-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)

10/560012



RN 115416-50-7 ZCAPLUS
CN 1-Propanol, 3-[[4-nitro-3-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)



L70 ANSWER 32 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:103817 ZCAPLUS Full-text
DOCUMENT NUMBER: 96:103817
ORIGINAL REFERENCE NO.: 96:17037a,17040a
TITLE: Nitrating anilides
INVENTOR(S): Peer, Lydia; Mayer, Joseph
PATENT ASSIGNEE(S): Schering Corp., USA
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 4302599	A	19811124	US 1979-73838	19790910 <--
PRIORITY APPLN. INFO.:			US 1979-73838	19790910 <--
OTHER SOURCE(S):	MARPAT 96:103817			

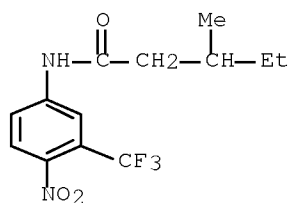
AB Meta-substituted N-acylanilines reacted with HNO₃-oleum mixts. at between -20 and +50° to yield p-nitro-N-acylanilines. Thus, 3-F₃CC₆H₄NHCOCHMe₂ was added slowly to oleum at .apprx.5°, 90% HNO₃ was added dropwise, and the mixture was stirred 2 h at .apprx.5° to give 3,4-F₃C(O₂N)C₆H₃NHCOCHMe₂. The products are useful as bactericides, herbicides, and antiandrogenic agents (no data).

IT 80945-17-1F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 80945-17-1 ZCAPLUS

CN Pentanamide, 3-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L70 ANSWER 33 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1981:586828 ZCAPLUS Full-text

DOCUMENT NUMBER: 95:186828

ORIGINAL REFERENCE NO.: 95:31169a,31172a

TITLE: N,N-Disubstituted p-phenylenediamine derivatives

INVENTOR(S): Wollemann, Bruno; Haertner, Harrtmut; Bardonner, Hans

PATENT ASSIGNEE(S): Merck Patent G.m.b.H. , Fed. Rep. Ger.

SOURCE: Ger. Offen., 17 pp.

CODEN: GWXXBX

DOCUMENT TYPE: ~~Patent~~

LANGUAGE: German

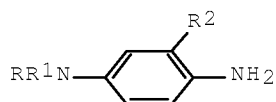
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

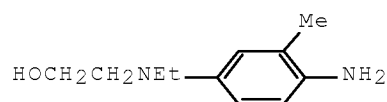
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2951100	A1	19810702	DE 1979-2951100	19791219 <--
DE 2951100	C2	19830210		
FR 2471967	A1	19810626	FR 1980-26664	19801216 <--
FR 2471967	B1	19840316		
GB 2065657	A	19810701	GB 1980-40329	19801217 <--
GB 2065657	B	19830824		
JP 56095152	A	19810801	JP 1980-179116	19801219 <--
JP 63053981	B	19881026		
US 4474987	A	19841002	US 1982-365131	19820405 <--
PRIORITY APPLN. INFO.:			DE 1979-2951100	A 19791219 <--
			US 1980-218249	A1 19801219 <--

OTHER SOURCE(S): MARPAT 95:186828

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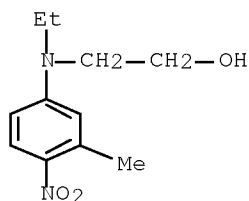


II

AB Title phenylenediamines I (R = C1-6 alkyl; R1 = C1-6 alkyl, sulfo- or alkylsulfonamidoalkyl; R2 = H, alkyl), useful as developers for color photog. (no data), were prepared Thus, 3-MeC6H4NEtCH2CH2OH was nitrosated with Me2CHONO, and the nitroso compound hydrogenated over Pd/C to give II (as the sulfate monohydrate).

10/560012

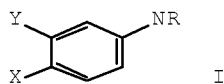
IT 52177-13-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrogenation of)
 RN 52177-13-6 ZCAPLUS
 CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 34 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1981:575793 ZCAPLUS Full-text
 DOCUMENT NUMBER: 95:175793
 ORIGINAL REFERENCE NO.: 95:29269a,29272a
 TITLE: Aniline derivatives as anti-testosterone drugs
 PATENT ASSIGNEE(S): Scherico Ltd., Switz.
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: ~~Patent~~
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56063916	A	19810530	JP 1980-87231	19800626 <--
JP 56049884	B	19811125	JP 1971-45301	19710624 <--
JP 58140052	A	19830819	JP 1982-161540	19820916 <--
PRIORITY APPLN. INFO.:			JP 1971-45301	A 19710624 <--
			DE 1971-2130450	A 19710619 <--
			JP 1980-87231	19800626 <--

GI



AB I (R = H or C1-4 alkyl, X = NO2 or Cl, Y = H, Me, CF3, F, or Cl, Z = H, COCHMe2, or other acyl groups) are synthesized as testosterone inhibitors. Thus, N-(isobutyryl)-4-nitro-3-trifluoromethylaniline (II) [13311-84-7] was prepared by treating 4-nitro-3-trifluoromethylaniline [393-11-3] with isobutyryl chloride [79-30-1]. Tablets were prepared by combining II 5, starch 5, lactose 89.5, and Mg stearate 0.5 mg/tablet.
 IT 39240-77-2P

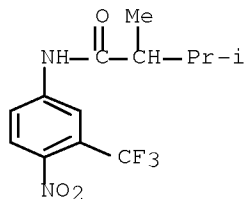
10/560012

RL: PREP (Preparation)

(preparation of, as testosterone inhibitor)

RN 39240-77-2 ZCAPLUS

CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 35 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1980:58461 ZCAPLUS Full-text

DOCUMENT NUMBER: 92:58461

ORIGINAL REFERENCE NO.: 92:9675a,9678a

TITLE: Cycloalkanecarboxanilide derivative herbicides

INVENTOR(S): Pilgram, Kurt H. G.; Skiles, Richard D.

PATENT ASSIGNEE(S): Shell Oil Co., USA

SOURCE: U.S., 5 pp.

CODEN: USXXAM

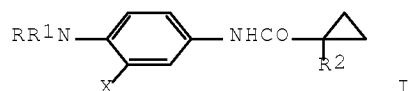
DOCUMENT TYPE: ~~Patent~~

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 7

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4168153	A	19790918	US 1978-876594	19780210 <--
CA 1087186	A1	19801007	CA 1978-294281	19780104 <--
BE 863074	A1	19780719	BE 1978-184445	19780119 <--
SE 7800692	A	19780722	SE 1978-692	19780119 <--
NL 7800656	A	19780725	NL 1978-656	19780119 <--
DE 2802282	A1	19780727	DE 1978-2802282	19780119 <--
JP 53092739	A	19780815	JP 1978-3778	19780119 <--
BR 7800354	A	19781010	BR 1978-354	19780119 <--
AU 7832543	A	19790726	AU 1978-32543	19780119 <--
AU 523765	B2	19820812		
AT 7800395	A	19800615	AT 1978-395	19780119 <--
AT 360799	B	19810126		
GB 1593932	A	19810722	GB 1978-2214	19780119 <--
CH 637917	A5	19830831	CH 1978-563	19780119 <--
PRIORITY APPLN. INFO.:			US 1977-761515	A2 19770121 <--
GI				

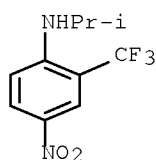


AB Seventeen cyclopropanecarboxanilides I (R = H, Me, Pr; R1 = H, Me, Me2CH, Me3C, cyclopropyl, 1-methylcyclopropyl, Pr; R2 = Me, Cl, Et; X = CF3, NO2, Br, Me) were prepared by acylation of the appropriate aniline with a cyclopropanecarbonyl chloride. Tests with 15 I showed both pre- and postemergence herbicidal activity. Thus, acylation of 4,3-(Me2CHNH)(F3C)C6H3NH2 with 1-methylcyclopropanecarbonyl chloride gave 84% I (R = H, R1 = Me2CH, R2 = Me, X = CF3).

IT 70339-08-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and reduction of nitro group in)

RN 70339-08-1 ZCAPLUS

CN Benzenamine, N-(1-methylethyl)-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 36 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:523221 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 91:123221

ORIGINAL REFERENCE NO.: 91:19879a,19882a

TITLE: Dipole moment study of the ortho-effect in
 4-substituted NN-dimethyl-2-trifluoromethylanilines

AUTHOR(S): Hallas, Geoffrey; Hepworth, John D.; Jones, Peter;
 Ibbitson, Douglas A.; Jones, Alan M.; Turton, Andrew
 R.

CORPORATE SOURCE: Dep. Colour Chem., Leeds Univ., Leeds, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions
 2: Physical Organic Chemistry (1972-1999) (1979),
 (4), 525-8

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

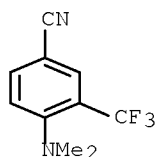
AB Apparent dipole moments of 4,2-R(CF3)C6H3NMe2 (R = H, Me, Cl, Br, iodo, cyano, O2N, Me2N, H2N) in C6H6 were determined. Vector moments in the direction of the major axis of the ring were calculated to explain the observed dipole moments. These vector moments are compared with corresponding values calculated for 4-RC6H4NMe2 (R = Cl, Br, iodo, cyano, O2N). The influence of the 2-CF3 group on the extent to which para substitution restores conjugation between the Me2N group and the ring is noted.

IT 71145-96-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and ortho effect in, dipole moment study of)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 37 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:490927 ZCAPLUS Full-text

DOCUMENT NUMBER: 91:90927

ORIGINAL REFERENCE NO.: 91:14683a,14686a

TITLE: Evidence for electronic buttressing in 4-substituted NN-dimethyl-2-trifluoromethylanilines: long range fluorine-19-proton coupling

AUTHOR(S): Bartle, Keith D.; Hallas, Geoffrey; Hepworth, John D.; Jones, Peter; Matthews, Raymond S.

CORPORATE SOURCE: Dep. Phys. Chem., Univ. Leeds, Leeds, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1979), (2), 192-4

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ¹H NMR spectra of fourteen 4,2-R(F3C)C6H4NMe2 were examined. A long range ¹⁹F-¹H coupling 6J(F,H) between NMe and CF3 was confirmed by ¹⁹F NMR. A linear relation holds between 6J(F,H) in these compds. and the appropriate Hammett para substituent consts. in accord with the operation of electronic buttressing; a similar correlation holds between the chemical shift of the N-Me protons and σ_p .

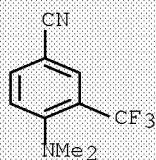
IT 71145-96-5

RL: PRP (Properties)

(NMR of, electronic buttressing in relation to)

RN 71145-96-5 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-3-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 38 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:203718 ZCAPLUS Full-text

DOCUMENT NUMBER: 90:203718

ORIGINAL REFERENCE NO.: 90:32397a,32400a

TITLE: Cycloalkanecarboxanilides with herbicide activity

INVENTOR(S): Pilgram, Kurt H. G.; Skiles, Richard D.

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.

SOURCE: Fr. Demande, 57 pp.

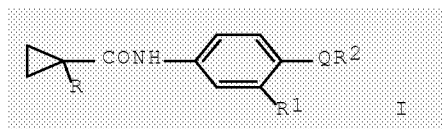
CODEN: FRXXBL

10/560012

DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 7
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2377999	A1	19780818	FR 1978-1493	19780119 <--
FR 2377999	B1	19810327		
CA 1087186	A1	19801007	CA 1978-294281	19780104 <--
BE 863074	A1	19780719	BE 1978-184445	19780119 <--
SE 7800692	A	19780722	SE 1978-692	19780119 <--
NL 7800656	A	19780725	NL 1978-656	19780119 <--
DE 2802282	A1	19780727	DE 1978-2802282	19780119 <--
JP 53092739	A	19780815	JP 1978-3778	19780119 <--
BR 7800354	A	19781010	BR 1978-354	19780119 <--
AU 7832543	A	19790726	AU 1978-32543	19780119 <--
AU 523765	B2	19820812		
AT 7800395	A	19800615	AT 1978-395	19780119 <--
AT 360799	B	19810126		
GB 1593932	A	19810722	GB 1978-2214	19780119 <--
CH 637917	A5	19830831	CH 1978-563	19780119 <--
PRIORITY APPLN. INFO.:			US 1977-761515	A 19770121 <--

GI



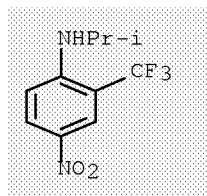
AB Ninety-four herbicidal I (R = C1-6 alkyl, Cl, F, Br, alkoxy or alkylthio; R1 = halo, CN, NO2, CR3:NOR3, COR3, Q1R3; R2 = optionally halogenated alkyl, alkenyl or aryl, alkynyl, alkoxyalkyl, etc.; R3 = H, alkyl or cycloalkyl; Q = O, S, SO, SO2 or NR3; Q1 = O, S, SO or SO2) were prepared; extensive data for both pre- and postemergence application are given. Thus, 3,4-(F3C)ClC6H3NO2 was treated with Me2CHONa, the NO2 group was reduced, and the aniline was acylated with 1-methylcyclopropanecarbonyl chloride to give I (R = Me, R1 = Cl, R2 = Me2CH, Q = O).

IT 70339-08-1F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)

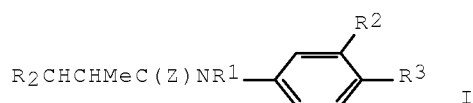
RN 70339-08-1 ZCAPLUS

CN Benzenamine, N-(1-methylethyl)-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 39 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1978:22155 ZCAPLUS Full-text
 DOCUMENT NUMBER: 88:22155
 ORIGINAL REFERENCE NO.: 88:3549a,3552a
 TITLE: Alkanoic acid anilides
 INVENTOR(S): Neri, Rudolph O.; Topliss, John G.
 PATENT ASSIGNEE(S): Scherico Ltd., Switz.
 SOURCE: Can., 56 pp.
 CODEN: CAXXA4
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CA 1012462	A1	19770621	CA 1971-116108	19710618 <--
PRIORITY APPLN. INFO.:			CA 1971-116108	A 19710618 <--
GI				



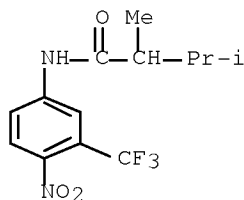
AB Eight alkanolic anilides I (Z = O, S; R = H, Me; R1 = H, Me, Et; R2 = CF3, Cl, Br; R3 = NO2, Cl), which are useful as anti-androgenic agents (no data), were prepared by various methods. Amidation of Me2CHCOCl by an aniline derivative yielded I (Z = O, R = R1 = H, R2 = CF3, R3 = NO2). The Beckmann rearrangement of 4,3-Cl(F3C)C6H3C(:NOH)CHMe2 gave I (R = R1 = H, R2 = CF3, R3 = Cl, Z = O). I (R = R1 = H, R2 = CF3, R3 = NO2, Z = S) was prepared from Me2CHCS2Me and the resp. aniline.

IT 39240-77-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

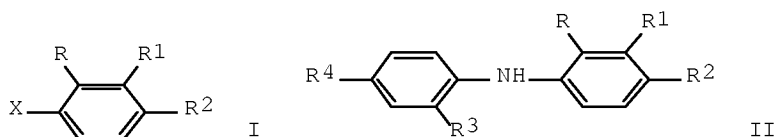
RN 39240-77-2 ZCAPLUS

CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

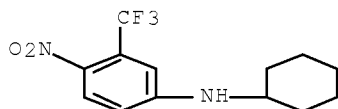


10/560012

L70 ANSWER 40 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1977:189358 ZCAPLUS Full-text
 DOCUMENT NUMBER: 86:189358
 ORIGINAL REFERENCE NO.: 86:29689a,29692a
 TITLE: Synthesis of 4-aminodiphenylamine and its relatives
 AUTHOR(S): Rondestvedt, Christian S., Jr.
 CORPORATE SOURCE: Jackson Lab., E. I. Du Pont de Nemours and Co.,
 Wilmington, DE, USA
 SOURCE: Journal of Organic Chemistry (1977), 42(10), 1786-90
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 86:189358
 GI



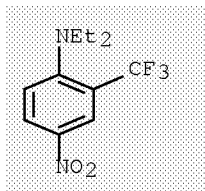
AB Formanilides and acetanilides condensed with halonitrobenzenes I (R = NO₂, H, Cl; R₂ = H, CF₃; R₃ = H, Me, NO₂; X = Cl, F) to give eight resp. diphenylamines II (R₃ = H, Me; R₄ = H, OEt).
 IT 61587-18-6P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 61587-18-6 ZCAPLUS
 CN Benzenamine, N-cyclohexyl-4-nitro-3-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 41 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1975:409343 ZCAPLUS Full-text
 DOCUMENT NUMBER: 83:9343
 ORIGINAL REFERENCE NO.: 83:1545a,1548a
 TITLE: Substituted N,N-dimethylanilines containing an o-trifluoromethyl group. Synthesis of N,N-dimethyl-2-trifluoromethylaniline
 AUTHOR(S): Hepworth, John D.; Jones, Peter; Hallas, Geoffrey
 CORPORATE SOURCE: Div. Chem., Polytech. Preston, Preston, UK
 SOURCE: Synthesis (1974), (12), 874-6
 CODEN: SYNTBF; ISSN: 0039-7881
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 83:9343

10/560012

GI For diagram(s), see printed CA Issue.
 AB The amines I (X = Me2N, MeNH, piperidino, morpholino, Et2N) were prepared in 74-94% yield by the reaction of I (X = Cl) with the corresponding amine. Reduction of I (X = Me2N) gave 94% 4,2-H2N(F3C)C6H3NMe2 (II), which was converted to its Ac and Bz derivs. Diazotization of II followed by treatment with CuBr in HBr gave 91% 4,2-Br(F3C)C6H3NMe2, which when treated with BuLi gave 72% 2-F3CC6H4NMe2.
 IT 25900-35-0F
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 25900-35-0 ZCAPLUS
 CN Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 42 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1974:425336 ZCAPLUS Full-text
 DOCUMENT NUMBER: 81:25336
 ORIGINAL REFERENCE NO.: 81:4085a,4088a
 TITLE: p-Nitroaniline derivatives
 INVENTOR(S): Suda, Hideaki; Kanda, Tatsuo; Tomita, Hiroshige;
 Nakanishi, Hirotoshi; Hida, Hiroshi; Nuno, Tatsumi
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49020129	A	19740222	JP 1972-63507	19720623 <--
CA 1012553	A1	19770621	CA 1973-174587	19730621 <--
DE 2331900	A1	19740124	DE 1973-2331900	19730622 <--
DE 2331900	C2	19861113		
FR 2199533	A1	19740412	FR 1973-22956	19730622 <--
IT 991637	B	19750830	IT 1973-68879	19730622 <--
GB 1421600	A	19760121	GB 1973-29902	19730622 <--
CH 593236	A5	19771130	CH 1973-9211	19730625 <--
FR 2225423	A1	19741108	FR 1974-3932	19740206 <--
FR 2225423	B1	19780616		
PRIORITY APPLN. INFO.:			JP 1972-18191	A 19720213 <--
			JP 1972-63507	A 19720623 <--
			JP 1972-63508	A 19720623 <--
			JP 1972-63509	A 19720623 <--
			JP 1972-63512	A 19720623 <--
			JP 1972-63513	A 19720623 <--
			JP 1972-64714	A 19720627 <--
			JP 1972-66286	A 19720701 <--
			JP 1973-18191	A 19730213 <--

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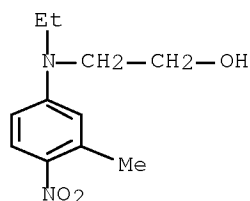
GI For diagram(s), see printed CA Issue.

AB The nitroanilines (I; R1, R2 = H, C1-6alkyl, CH2CH2OH, CH2CH2Cl, β -acylaminoethyl, CH2CH2NHSO2Me, but not R1 = R2 = H) were prepared by treating the nitrophenol ethers (II; R3 = C1-6 alkyl, Ph) with HNR1R2. Thus, heating II (R3 = Me) with 15 mole 20% aqueous EtNH2 at 180° for 10 hr gave 97% I (R1 = Et, R2 = H) with 93% conversion. Among 5 more I prepared were the following (R1, R2 given): Pr, H; CH2CH2OH, H; CH2CH2OH, Et; CH2CH2NHSO2Me, Et.

IT ~~52177-13-6P~~
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 52177-13-6 ZCAPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



L70 ANSWER 43 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:108165 ZCAPLUS Full-text

DOCUMENT NUMBER: 80:108165

ORIGINAL REFERENCE NO.: 80:17387a,17390a

TITLE: N,N-Disubstituted p-phenylenediamines

INVENTOR(S): Suda, Hideaki; Kanda, Tatsuo; Tomita, Hiroshige; Nakanishi, Hirotoshi; Hida, Himoru; Nuno, Tatsuli

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.

SOURCE: Ger. Offen., 53 pp.
 CODEN: GWXXBX

DOCUMENT TYPE: ~~Patent~~

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 2331900	A1	19740124	DE 1973-2331900	19730622 <--
DE 2331900	C2	19861113		
JP 49020129	A	19740222	JP 1972-63507	19720623 <--
JP 49020130	A	19740222	JP 1972-63508	19720623 <--
JP 51024491	B	19760724		
JP 49020131	A	19740222	JP 1972-63512	19720623 <--
JP 51040061	B	19761101		
JP 49020128	A	19740222	JP 1972-63513	19720623 <--
JP 55008501	B	19800304	JP 1972-63509	19720623 <--
JP 49020133	A	19740222		
JP 49024924	A	19740305	JP 1972-64714	19720627 <--
JP 55010577	B	19800317		
JP 49024923	A	19740305	JP 1972-66286	19720701 <--
JP 49102629	A	19740927	JP 1973-18191	19730213 <--
JP 52005486	B	19770214		
US 3920739	A	19751118	US 1973-378059	19730711 <--

10/560012

PRIORITY APPLN. INFO.:

JP 1972-63507	A	19720623	<--
JP 1972-63508	A	19720623	<--
JP 1972-63509	A	19720623	<--
JP 1972-63512	A	19720623	<--
JP 1972-63513	A	19720623	<--
JP 1972-64714	A	19720627	<--
JP 1972-66286	A	19720701	<--
JP 1973-18191	A	19730213	<--

GI For diagram(s), see printed CA Issue.

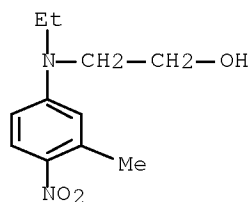
AB Four diamines I (R = H, Me; R1 = Et, CH₂CH₂OMe, CH₂CH₂NHSO₂Me) were prepared in ≤100% yield by alkylation of II and subsequent reaction with R₁NHEt or successively with EtNH₂ and R₁X (X = Cl, OH), or with EtNH₂, ClSO₂Me, and HOCH₂CH₂NH₂ followed by reduction over Pd/C.

IT 52177-13-6P 52177-25-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

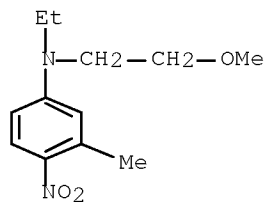
RN 52177-13-6 ZCAPLUS

CN Ethanol, 2-[ethyl(3-methyl-4-nitrophenyl)amino]- (CA INDEX NAME)



RN 52177-25-0 ZCAPLUS

CN Benzenamine, N-ethyl-N-(2-methoxyethyl)-3-methyl-4-nitro- (CA INDEX NAME)



L70 ANSWER 44 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1974:61050 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 80:61050

ORIGINAL REFERENCE NO.: 80:9905a,9908a

TITLE: Steric effects in di- and triarylmethane dyes. XI.
Electronic absorption spectra of derivatives of
Michler's hydrol blue, crystal violet, and malachite
green containing o-trifluoromethyl groups

AUTHOR(S): Grocock, D. E.; Hallas, G.; Hepworth, J. D.

CORPORATE SOURCE: Dep. Sci., North Lindsay Coll. Technol., Scunthorpe,
UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (1972-1999) (1973),
(13), 1792-6
CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

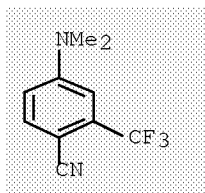
AB The effects of substitution of o-CF₃ groups in Michler's hydrol blue [14844-71-4], crystal violet [548-62-9], and malachite green [569-64-2] were examined. Bathochromic shifts of the first bands were observed for electronically sym. dyes. Addition of a CF₃ group at the 2'-position of malachite green produced a conformational change which caused a hypsochromic shift of the first band. In certain cases, the combined steric and electronic effects of the CF₃ groups were enough to shift the equilibrium between dye base and univalent dye cation in acid solution in favor of the former species.

IT 51332-25-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 51332-25-3 ZCAPLUS

CN Benzonitrile, 4-(dimethylamino)-2-(trifluoromethyl)- (CA INDEX NAME)



L70 ANSWER 45 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:478429 ZCAPLUS Full-text
DOCUMENT NUMBER: 79:78429
ORIGINAL REFERENCE NO.: 79:12713a,12716a
TITLE: Antiandrogenic substituted anilides
PATENT ASSIGNEE(S): Scherico Ltd.
SOURCE: Fr. Demande, 40 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2142803	A1	19730202	FR 1971-23250	19710625 <--
FR 2142803	B1	19740830		

PRIORITY APPLN. INFO.: FR 1971-23250 A 19710625 <--

GI For diagram(s), see printed CA Issue.

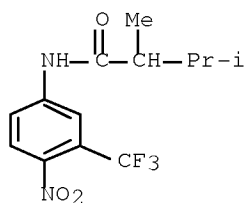
AB Ten anilides (I; R = CHMe₂, CHMeCHMe₂; R₁ = H, Me, Et; R₂ = CF₃, SOCF₃, Br, Cl; R₃ = NO₂, Cl), potential antiandrogenic agents, are prepared by thirteen standard methods.

IT 39240-77-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 39240-77-2 ZCAPLUS

CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 46 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1973:58091 ZCAPLUS Full-text
 DOCUMENT NUMBER: 78:58091
 ORIGINAL REFERENCE NO.: 78:9207a,9210a
 TITLE: Substituted anilides and thioanilides
 INVENTOR(S): Neri, Rudolph O.; Topliss, John G.
 PATENT ASSIGNEE(S): Scherico Ltd.
 SOURCE: Ger. Offen., 73 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

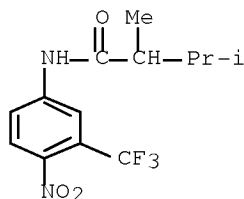
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2130450	A	19721221	DE 1971-2130450	19710619 <--
DE 2130450	B2	19771013		
JP 56049884	B	19811125	JP 1971-45301	19710624 <--
PRIORITY APPLN. INFO.:			DE 1971-2130450	A 19710619 <--

AB Nine anilides 3,4-RR1C6H3NR2CXR3 (I; R = Cl, F3C, F3CSO; R1 = Cl, O2N; R2 = H, Me, Et; R3 = CHMe2, CHMeCHMe2; X = O, S), useful antiandrogenic agents, were prepared mainly by acylation of 3,4-RR1C6H3NH2 (II). Thus, Me2CHCOCl was heated with II (R = F3C, R1 = O2N) in pyridine for 1.5 hr to give I (R = F3C, R1 = O2N, R2 = H, R3 = CHMe2, X = O).

IT 39240-77-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 39240-77-2 ZCAPLUS

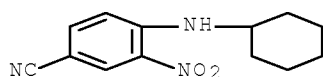
CN Butanamide, 2,3-dimethyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 47 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1970:121102 ZCAPLUS Full-text

10/560012

DOCUMENT NUMBER: 72:121102
ORIGINAL REFERENCE NO.: 72:21755a,21758a
TITLE: Antitubercular substances. XXI. Synthesis of 2-nitrodiphenylamines
AUTHOR(S): Belton, J. G.; McInerney, Mary
CORPORATE SOURCE: Lab. Med. Res. Counc. Ireland, Trinity Coll., Dublin, Ire.
SOURCE: Proceedings of the Royal Irish Academy, Section B: Biological, Geological and Chemical Science (1970), 69(2), 21-9
CODEN: PRIBAN; ISSN: 0035-8983
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) were prepared by heating halonitrobenzenes with anilines or cyclohexylamine, by treating nitroanilines with halobenzenes in the presence of anhydrous K₂CO₃, KIO₄, and reduced Cu, by treating dinitrobenzenes with haloanilines, or by replacing Cl with alkoxy, thioalkyl, or amido groups on a preformed diphenylamine. The following (I) were prepared (R₁, R₂, R, m.p., and % yield given): CN, H, Ph, 126° (alc.), -; F₃C, H, C₆H₁₁, 80-1° (light petroleum), 75; F₃C, H, Ph, 84-5° (alc.), 69; Et, H, Ph, 121° (MeOH), -; HO₂C, H, Ph, 220° (alc.), -; Cl, H, Ph, 61° (alc.), -; Cl, Cl, Ph, 96°, 61; H, H, 4-ClC₆H₄, 150°, 25; Cl, H, 3-MeOC₆H₄, 92-3°, 60; Cl, H, 4-MeOC₆H₄, 121°, 70; Cl, H, 3-EtOC₆H₄, 92°, 68; Cl, H, 4-EtOC₆H₄, 95°, 80; F, H, Ph, 53°, -; H, H, 3-MeOC₆H₄, 57-8° (alc.), 44; H, H, 4-MeOC₆H₄, 89°, 50; H, H, 3-EtOC₆H₄, 47.5-8.5° (alc.), 30; H, H, 4-EtOC₆H₄, 84°, 56; tert-Bu, H, Ph, 73-4° (alc.), -; EtO, H, Ph, 74°, 52; BuO, H, Ph, 57-8° (alc.), 40; EtO, H, 4-ClC₆H₄, 68-9° (alc.), -; Cl, H, 4-MeOC₆H₄, 112-14° (alc.) 40; MeO, H, 4-MeC₆H₄, 85-6° (alc.), 50; EtO, H, 4-MeC₆H₄, 75° (alc.), 50; H, H, 3-MeC₆H₄, 70-1° (MeOH), 71; H, Cl, 4-BrC₆H₄, 160-1° (C₆H₆-alc.), -; H, Cl, 3-ClC₆H₄, 109° (alc.), 30; H, Cl, 4-IC₆H₄, 186-7°, -; H, MeO, 4-BrC₆H₄, 149° (alc.), -; H, MeO, 4-IC₆H₄, 167° (alc.), 80-90; H, MeO, 3-ClC₆H₄, 107° (alc.), 80-90; Cl, MeO, Ph, 103-4° (alc.), 80-90; H, MeO, C₆H₁₁, 78-9° (alc.), 80-90; H, EtO, Ph, 107-8° (alc.), -; H, MeS, 4-ClC₆H₄ (II), 133° (alc.), -; H, MeS, Ph, 135° (alc.), -; H, phthalimido, Ph, 203-4°, -; H, NH₂, Ph, 126-7° (aqueous alc.), -; H, NHAc, Ph, 202-3°, -; Cl, C₆H₁₁, Ph, 124-5° (light petroleum), -. Na₂S₂, Na₂S.9H₂O, and S in 95% aqueous alc. were added to 5,4'-dichloro-2-nitrodiphenylamine in 95% aqueous alc. and HCONMe₂ and heated on a water bath 2 hr to give 3,3'-bis(p-chloroanilino)-4,4'-dinitrophenyl disulfide, yellow, m. 190-1° (HCONMe₂-alc.), which was used to prepare II.
IT ~~28096-55-1P~~
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 28096-55-1 ZCAPLUS
CN Benzonitrile, 4-(cyclohexylamino)-3-nitro- (CA INDEX NAME)

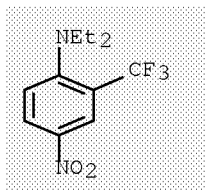


L70 ANSWER 48 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1970:66670 ZCAPLUS Full-text
DOCUMENT NUMBER: 72:66670

10/560012

ORIGINAL REFERENCE NO.: 72:12151a,12154a
 TITLE: Herbicidal alkylaminophenylureas
 INVENTOR(S): Schwartz, Herbert; Skaptason, Joseph B.
 SOURCE: U.S., 4 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3484484	A	19691216	US 1967-626409	19670328 <--
PRIORITY APPLN. INFO.:			US 1967-626409	A 19670328 <--
GI	For diagram(s), see printed CA Issue.			
AB	The title compounds (I) are useful as preemergent and postemergent herbicides. Thus, a mixture of 98 g 4-chloro-3-(trifluoromethyl)-nitrobenzene and 97 g Pr2NH in 150 ml MeOH was refluxed overnight to give 89 g II (R1 = R2 = Pr, X = CF3, Y = NO2), b0.5 86-9°, which was hydrogenated over Pd/C to give II (R1 = R2 = Pr, X = NH2), b1 85-8°, of which 14 g was dissolved in 150 ml C6H6, and 4.5 ml pyridine then 6 g Me2NCOCl added at room temperature to give I (R1 = R2 = Pr, X = CF3, R3 = Me), m. 124-5° (C6H6-C6H14). Similarly prepared were the tabulated I. Similarly prepared were II (R1 = R2 = Et, X = CF3, Y = NO2), b1 95-8°, and II (R1 = R2 = Pr, X = Cl, Y = NO2), m. 141-3°.			
IT	25900-35-0P			
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	25900-35-0 ZCAPLUS			
CN	Benzenamine, N,N-diethyl-4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)			



L70 ANSWER 49 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1969:87264 ZCAPLUS Full-text
 DOCUMENT NUMBER: 70:87264
 ORIGINAL REFERENCE NO.: 70:16285a,16288a
 TITLE: Nitro(trifluoromethyl)toluidides
 INVENTOR(S): Baker, Joseph W.
 PATENT ASSIGNEE(S): Monsanto Co.
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3426049	A	19690204	US 1965-497437	19651018 <--
PRIORITY APPLN. INFO.:			US 1965-497437	A 19651018 <--

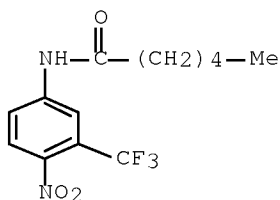
10/560012

AB The title compds. possessing useful microbiol. activity were prepared Thus, 0.055 mole valeryl chloride was added to 0.05 mole α,α,α -trifluoro-4-nitro-m-toluidine (I). The mixture was refluxed until the evolution of HCl ceased, 75 ml. methylcyclohexane added, and the mixture cooled to yield α,α,α -trifluoro-4'-nitro-m-valerotoluidide (IIa), m. 94-5°. Similarly prepared were RCONHC6H3(CF3)NO2-3,4 (RCO and m.p. given): isovaleryl, (IIb), 103-4°; 2-methylbutyryl, 111-12°; 4-methylvaleryl, 85-7°; hexanoyl (IIc), 73-4°; neoheptanoyl, 110.5-12°; decanoyl, 77-8°; undecanoyl, 82-3°; cyclopentanecarbonyl, 143-4°; cyclohexanecarbonyl, 135-6°; hydrocinnamoyl, 90.5-92°; sorboyl, 123-4°; 3-ethyl-2-hexanoyl, 90-1°; 2-nonenoyl, 59-60°; 2-bromononanoyl, 102-3°; 2-chlorononanoyl, 55-6°; nonanoyl (II), 69-70°; heptanoyl (III), 64-5°; octanoyl (IV), 72-3°; lauroyl, 78-9°; 10-undecenoyl, 77-8°; 2-nonynoyl, 47-8°. A solution of 0.05 mole nonanoyl chloride in 25 ml. ether was added to a solution of 0.05 mole I and 0.05 mole Et3N in 200 ml. ether. The mixture was refluxed for 3 hrs., cooled, and Et3N.-HCl removed to yield II-I complex, m. 84-5°. An excess of ethereal HCl was added to a solution of 10 g. II-I complex in 75 ml. ether and the toluidine-HCl removed to yield II. Similarly prepared were α,α,α -trifluoro-4-methyl-4'-nitro-m-valerotoluidide-I complex, m. 97-8°; III-I complex, m. 94-5°; IV-I complex, m. 90-1°. A solution of 0.0017 mole IIa and 0.0017 mole I in 10 ml. toluene-methylcyclohexane mixture was cooled to give IIa-I complex, m. 96-7°. Similarly prepared were IIb-I complex, m. 103-4°; IIc-I complex, m. 106-7°. A solution of 0.014 mole Br in 25 ml. CCl4 was added to a solution of 0.014 mole α,α,α -trifluoro-4'-nitro-m-(2-noneno)toluidide in 100 ml. CCl4 at 0-5°, the mixture kept 6 hrs. at 0-5°, 1.5 g. KOAc in 10 ml. EtOH added, and the mixture refluxed 30 min. to give 2,3-dibromo- α,α,α -trifluoro-4'-nitro-m-nonanotoluidide, m. 107-8°.

IT 10023-90-2P 10023-91-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

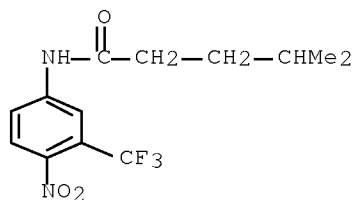
RN 10023-90-2 ZCAPLUS

CN Hexanamide, N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 10023-91-3 ZCAPLUS

CN Pentanamide, 4-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 50 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:37593 ZCAPLUS Full-text

DOCUMENT NUMBER: 66:37593

ORIGINAL REFERENCE NO.: 66:7131a, 7134a

TITLE: Synthesis and bacteriostatic activity of some nitrotrifluoromethylanilides

AUTHOR(S): Baker, Joseph Willard; Bachman, Gerald L.; Schumacher, Ignatius; Roman, Daniel P.; Tharp, Alan L.

CORPORATE SOURCE: Org. Chems. Div., Monsanto Co., St. Louis, MO, USA

SOURCE: Journal of Medicinal Chemistry (1967), 10(1), 93-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

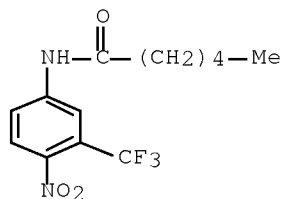
AB Nitrotrifluoromethylanilides (I) were prepared either by the acid-catalyzed reaction of an anhydride with a substituted aniline or by the condensation of an acid chloride or with the aniline alone or in the presence of Et3N as the HCl acceptor. Seven anilide-aniline complexes were formed when C5-9 acid chlorides free of α -substituents were treated with 4-nitro-3-trifluoromethylaniline in the presence of Et3N. The active structures of the nitrotrifluoromethylanilides which inhibited the activity of Staphylococcus aureus included those which were substituted in the meta and para positions of the N-phenyl ring with a nitro and trifluoromethyl group and in which the acid-derived moiety incorporates alkyl, haloalkyl, cycloalkyl, alkenyl, haloalkenyl, alkylidenyl, and phenethyl groups and contains 5-12 C atoms. Anilides substituted in the α position possessed a lower order of activity. Benzyl and phenoxyethyl derivs. and disubstituted and orthosubstituted derivs. were inactive. All of the complexes were derivs. of active anilides and exhibited the same order of activity on a weight basis as the anilides themselves.

IT 10023-90-2P 10023-91-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

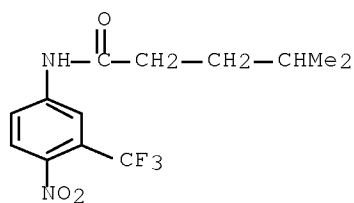
RN 10023-90-2 ZCAPLUS

CN Hexanamide, N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



10/560012

RN 10023-91-3 ZCAPLUS
CN Pentanamide, 4-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L70 ANSWER 51 OF 51 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1942:29161 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 36:29161

ORIGINAL REFERENCE NO.: 36:4490c-f

TITLE: Alkanolamines. X. Intermediates of pentryl analogs.
Chloronitroanilinoalkanols

AUTHOR(S): Kremer, Chester B.; Meltsner, M.

SOURCE: Journal of the American Chemical Society (1942), 64,
1285-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 34, 6942.2. The condensations were carried out by refluxing for 4 h. the Cl2C6H3NO2 and twice the mol. quantity of the NH2 alc. in BuOH. 2-(R-anilino)ethanols (R given): 4-chloro-2-nitro, m. 107.5°; 5-Cl isomer, m. 116°; 3-Cl isomer, m. 78.5°; 6-Cl isomer, b2 155-7°; 6-chloro-4-nitro, m. 120°. 3-(R-anilino)-1-propanols: 4-chloro-2-nitro, m. 60°; 5-Cl isomer, m. 78.5°; 6-chloro-4-nitro, m. 73°. 1-(R-anilino)-2-propanols: 4-chloro-2-nitro, m. 116.5°; 5-Cl isomer, m. 109°; 3-Cl isomer, m. 83.5°; 6-chloro-4-nitro, m. 144°. 1-(R-anilino)-2-methyl-2-propanols: 4-chloro-2-nitro, m. 121.5°; 5-Cl isomer, m. 127°; 3-Cl isomer, m. 98.5°; 6-chloro-4-nitro, m. 71.5°. 2-(4-Chloro-2-nitroanilino)-2-methyl-1-propanol, m. 122°. Reduction was effected with NaHSO3 in a weakly alkaline medium: 2-(R-2-aminoanilino)ethanols: 4-Cl, m. 122.5°; 5-Cl, m. 104.5°; 3-Cl, m. 74°; 6-Cl, b2 135-7°. 3-(5-Chloro-2-aminoanilino)-1-propanol, m. 73.5°. 1-(4-Chloro-2-aminoanilino)-2-propanol, m. 130°; 5-Cl isomer, m. 101.5°. 1-(4-Chloro-2-aminoanilino)-2-methyl-2-propanol, m. 121°; 2-(4-chloro-2-aminoanilino)-2-methyl-1-propanol.

IT ~~854666-45-8P~~, 2-Propanol, 1-(2-chloro-4-nitroanilino)-2-methyl-

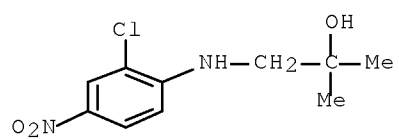
RL: PREP (Preparation)

(preparation of)

RN 854666-45-8 ZCAPLUS

CN 2-Propanol, 1-[(2-chloro-4-nitrophenyl)amino]-2-methyl- (CA INDEX NAME)

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FILE 'ZCAPLUS' ENTERED AT 08:39:33 ON 12 MAR 2009

ACT BAS012APP/A

L1 1 SEA SPE=ON ABB=ON PLU=ON US2005-560012 /AP

FILE 'REGISTRY' ENTERED AT 08:39:39 ON 12 MAR 2009

ACT BAS012APPRNS/A

L2 186 SEA SPE=ON ABB=ON PLU=ON (101130-93-2/BI OR 106-95-6/BI OR 106-96-7/BI OR 107-08-4/BI OR 107-10-8/BI OR 109-89-7/BI OR 115416-50-7/BI OR 142-84-7/BI OR 1458-98-6/BI OR 151951-35-8/BI OR 156-87-6/BI OR 1621-24-5/BI OR 194853-86-6/BI OR 208173-21-1/BI OR 2439-54-5/BI OR 24424-99-5/BI OR 2516-47-4/BI OR 26389-60-6/BI OR 2968-33-4/BI OR 31643-49-9/BI OR 393-09-9/BI OR 393-11-3/BI OR 393-36-2/BI OR 445-02-3/BI OR 4784-77-4/BI OR 49645-18-3/BI OR 513-49-5/BI OR 51332-25-3/BI OR 534-03-2/BI OR 5813-64-9/BI OR 625-43-4/BI OR 654-70-6/BI OR 67515-59-7/BI OR 7051-34-5/BI OR 75-64-9/BI OR 762-49-2/BI OR 821776-43-6/BI OR 821776-44-7/BI OR 821776-45-8/BI OR 821776-46-9/BI OR 821776-47-0/BI OR 821776-48-1/BI OR 821776-49-2/BI OR 821776-50-5/BI OR 821776-51-6/BI OR 821776-52-7/BI OR 821776-53-8/BI OR 821776-54-9/BI OR 821776-55-0/BI OR 821776-56-1/BI OR 821776-57-2/BI OR 821776-58-3/BI OR 821776-59-4/BI OR 821776-60-7/BI OR 821776-61-8/BI OR 821776-62-9/BI OR 821776-63-0/BI OR 821776-64-1/BI OR 821776-65-2/BI OR 821776-66-3/BI OR 821776-67-4/BI OR 821776-68-5/BI OR 821776-69-6/BI OR 821776-70-9/BI OR 821776-71-0/BI OR 821776-72-1/BI OR 821776-73-2/BI OR 821776-74-3/BI OR 821776-75-4/BI OR 821776-76-5/BI OR 821776-77-6/BI OR 821776-78-7/BI OR 821776-79-8/BI OR 821776-80-1/BI OR 821776-81-2/BI OR 821776-82-3/BI OR 821776-83-4/BI OR 821776-84-5/BI OR 821776-85-6/BI OR 821776-86-7/BI OR 821776-87-8/BI OR 821776-88-9/BI OR 821776-89-0/BI OR 821776-90-3/BI OR 821776-91-4/BI OR 821776-92-5/BI OR 821776-93-6/BI OR 821776-94-7/BI OR 821776-95-8/BI OR 821776-96-9/BI OR 821776-97-0/BI OR 821776-98-1/BI OR 821776-99-2/BI OR 821777-00-8/BI OR 821777-01-9/BI OR 821777-02-0/BI OR 821777-03-1/BI OR 821777-04-2/BI OR 821777-05-3/BI OR 821777-06-4/BI OR 821777-07-5/BI OR 821777-08-6/BI OR 821777-09-7/BI OR 821777

ACT BAS012HITRNS/A

L3 151 SEA SPE=ON ABB=ON PLU=ON (101130-93-2/BI OR 115416-50-7/BI OR 151951-35-8/BI OR 49645-18-3/BI OR 51332-25-3/BI OR 821776-43-6/BI OR 821776-44-7/BI OR 821776-45-8/BI OR 821776-46-9/BI OR 821776-47-0/BI OR 821776-48-1/BI OR 821776-49-2/BI OR 821776-50-5/BI OR 821776-51-6/BI OR 821776-52-7/BI OR 821776-53-8/BI OR 821776-54-9/BI OR 821776-55-0/BI OR 821776-56-1/BI OR 821776-57-2/BI OR 821776-58-3/BI OR 821776-59-4/BI OR 821776-60-7/BI OR 821776-61-8/BI OR 821776-62-9/BI OR 821776-63-0/BI OR 821776-64-1/BI OR 821776-65-2/BI OR 821776-66-3/BI OR 821776-67-4/BI OR 821776-68-5/BI OR 821776-69-6/BI OR 821776-70-9/BI OR

821776-71-0/BI OR 821776-72-1/BI OR 821776-73-2/BI OR 821776-74-3/BI OR 821776-75-4/BI OR 821776-76-5/BI OR 821776-77-6/BI OR 821776-78-7/BI OR 821776-79-8/BI OR 821776-80-1/BI OR 821776-81-2/BI OR 821776-82-3/BI OR 821776-83-4/BI OR 821776-84-5/BI OR 821776-85-6/BI OR 821776-86-7/BI OR 821776-87-8/BI OR 821776-88-9/BI OR 821776-89-0/BI OR 821776-90-3/BI OR 821776-91-4/BI OR 821776-92-5/BI OR 821776-93-6/BI OR 821776-94-7/BI OR 821776-95-8/BI OR 821776-96-9/BI OR 821776-97-0/BI OR 821776-98-1/BI OR 821776-99-2/BI OR 821777-00-8/BI OR 821777-01-9/BI OR 821777-02-0/BI OR 821777-03-1/BI OR 821777-04-2/BI OR 821777-05-3/BI OR 821777-06-4/BI OR 821777-07-5/BI OR 821777-08-6/BI OR 821777-09-7/BI OR 821777-10-0/BI OR 821777-11-1/BI OR 821777-12-2/BI OR 821777-13-3/BI OR 821777-14-4/BI OR 821777-15-5/BI OR 821777-16-6/BI OR 821777-17-7/BI OR 821777-18-8/BI OR 821777-19-9/BI OR 821777-20-2/BI OR 821777-21-3/BI OR 821777-22-4/BI OR 821777-23-5/BI OR 821777-24-6/BI OR 821777-25-7/BI OR 821777-26-8/BI OR 821777-27-9/BI OR 821777-28-0/BI OR 821777-29-1/BI OR 821777-30-4/BI OR 821777-31-5/BI OR 821777-32-6/BI OR 821777-33-7/BI OR 821777-34-8/BI OR 821777-35-9/BI OR 821777-36-0/BI OR 82177

ACT BAS012OLDRNS/A

L4 (1)SEA SPE=ON ABB=ON PLU=ON 49645-18-3
L5 (1)SEA SPE=ON ABB=ON PLU=ON 51332-25-3
L6 (1)SEA SPE=ON ABB=ON PLU=ON 96795-43-6
L7 (1)SEA SPE=ON ABB=ON PLU=ON 101130-93-2
L8 (1)SEA SPE=ON ABB=ON PLU=ON 115416-50-7
L9 (1)SEA SPE=ON ABB=ON PLU=ON 151951-35-8
L10 6 SEA SPE=ON ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8 OR L9)

D SCA

FILE 'STNGUIDE' ENTERED AT 08:41:38 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 08:45:14 ON 12 MAR 2009

L*** DEL 5594 S MG/ELS (P) BR/ELS

L*** DEL 1 S ?GRIGNARD?/CNS

D SCA

FILE 'STNGUIDE' ENTERED AT 08:51:02 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 09:22:39 ON 12 MAR 2009

D SCA L10

L11 3 SEA SPE=ON ABB=ON PLU=ON L10 AND X/ELS

FILE 'ZCAPLUS' ENTERED AT 09:23:07 ON 12 MAR 2009

L12 12 SEA SPE=ON ABB=ON PLU=ON L11

FILE 'REGISTRY' ENTERED AT 09:23:40 ON 12 MAR 2009

L13 STRUCTURE UPLOADED

L14 SCREEN 616

L15 151 SEA SPE=ON ABB=ON PLU=ON L11 OR L3

L16 0 SEA SPE=ON ABB=ON PLU=ON L15 AND C>21

L17 SCREEN 1951

L18 3 SEA SSS SAM L13 AND L14

L19 6 SEA SSS SAM L13 AND (L14 NOT L17)

D SCA

FILE 'STNGUIDE' ENTERED AT 09:31:23 ON 12 MAR 2009

10/560012

FILE 'REGISTRY' ENTERED AT 09:46:40 ON 12 MAR 2009
D SCA L19

FILE 'STNGUIDE' ENTERED AT 09:52:26 ON 12 MAR 2009

FILE 'REGISTRY' ENTERED AT 10:01:51 ON 12 MAR 2009

L20 STRUCTURE UPLOADED
L21 0 SEA SSS SAM L20
L22 1 SEA SSS SAM L20 AND (L14 NOT L17)
D SCA
L23 SCREEN 2043
L24 SCREEN 2043 OR 1951
L25 2 SEA SSS SAM L20 AND (L14 NOT L24)
D SCA
L26 STRUCTURE UPLOADED
L27 SCREEN 1993
L28 1 SEA SSS SAM L26 AND ((L14 AND L27) NOT L24)
D SCA
L29 0 SEA SPE=ON ABB=ON PLU=ON L3 AND NRS>2
L30 29 SEA SPE=ON ABB=ON PLU=ON L3 AND 2/NRS
D SCA L30
L31 SCREEN 1840
L32 SCREEN 1840 OR 2043 OR 1951
L33 2 SEA SSS SAM L26 AND ((L14 AND L27) NOT L32)
D SCA
L34 ANALYZE PLU=ON L30 1- RID : 4 TERMS
D
L35 898352 SEA SPE=ON ABB=ON PLU=ON (N>1 AND ((46.150.18/RID AND
1/NRS) OR (46.150.18/RID AND (1.13.1/RID OR 16.127.1/RID OR
46.150.1/RID) AND 2/NRS))) NOT PMS/CI
L36 7 SEA SUB=L35 SSS SAM L26 AND ((L14 AND L27) NOT L32)
D SCA
L37 8 SEA SUB=L3 SSS SAM L26 AND ((L14 AND L27) NOT L32)
D SCA
L38 1054 SEA SUB=L35 SSS FUL L26 AND ((L14 AND L27) NOT L32)
SAVE TEMP L38 BAS012STR26L/A

FILE 'ZCAPLUS' ENTERED AT 10:25:21 ON 12 MAR 2009

L39 3024 SEA SPE=ON ABB=ON PLU=ON L38

FILE 'REGISTRY' ENTERED AT 10:26:04 ON 12 MAR 2009

L40 1054 SEA SPE=ON ABB=ON PLU=ON L38 AND C<22
L41 143 SEA SPE=ON ABB=ON PLU=ON L3 AND C>10
L42 8 SEA SPE=ON ABB=ON PLU=ON L3 NOT L41
D SCA
L43 994 SEA SPE=ON ABB=ON PLU=ON L38 AND C>8

FILE 'ZCAPLUS' ENTERED AT 10:28:08 ON 12 MAR 2009

L44 2557 SEA SPE=ON ABB=ON PLU=ON L43

FILE 'REGISTRY' ENTERED AT 10:28:34 ON 12 MAR 2009

L45 97 SEA SPE=ON ABB=ON PLU=ON L3 AND F/ELS
L46 54 SEA SPE=ON ABB=ON PLU=ON L3 NOT L45
L47 135 SEA SPE=ON ABB=ON PLU=ON L38 AND L3
L48 16 SEA SPE=ON ABB=ON PLU=ON L3 NOT L47
D SCA
L49 0 SEA SPE=ON ABB=ON PLU=ON L47 AND BR/ELS
L50 1 SEA SPE=ON ABB=ON PLU=ON L48 AND BR/ELS AND 9/F
D SCA

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L51      10 SEA SPE=ON  ABB=ON  PLU=ON  L48 NOT BR/ELS
          D SCA
L52      6 SEA SPE=ON  ABB=ON  PLU=ON  L51 AND F/ELS
L53      7 SEA SPE=ON  ABB=ON  PLU=ON  L50 OR L52
L54     142 SEA SPE=ON  ABB=ON  PLU=ON  L47 OR L53
          D COST
          SEL RN
          SEL MF
          D COST FULL
L55     65815 SEA SPE=ON  ABB=ON  PLU=ON  (C14H19N3O2/MF OR C13H17N3O2/MF OR
          C12H13F3N2/MF OR C13H12F6N2O/MF OR C13H13N3O2/MF OR C15H19F3N2/
          MF OR C11H11F3N2O2/MF OR C11H8F6N2/MF OR C12H11F3N2/MF OR
          C13H15F3N2/MF OR C13H15N3O2/MF OR C13H16N2O2/MF OR C13H17CLN2/M
          F OR C13H17N3O3/MF OR C13H20N2O2/MF OR C14H14F6N2/MF OR
          C14H15F3N2O/MF OR C14H17F3N2/MF OR C14H17F3N2O2/MF OR C14H17N3O
          2/MF OR C15H17F3N2/MF OR C15H17F3N2O/MF OR C15H17N3O2/MF OR
          C15H19F3N2O/MF OR C15H19F3N2O2/MF OR C16H17F3N2/MF OR C16H21F3N
          2/MF OR C10H11F3N2O2/MF OR C10H11F3N2O3/MF OR C10H13CLN2O3/MF
          OR C10H6F6N2/MF OR C10H9F3N2/MF OR C11H11F3N2/MF OR C11H11F3N2O
          /MF OR C11H13F3N2O2/MF OR C11H13F3N2O3/MF OR C11H13N3O3/MF OR
          C11H15CLN2O2/MF OR C11H16CLN3O2/MF OR C11H16N2O3/MF OR
          C11H7BRF9N/MF OR C12H10F6N2/MF OR C12H10F6N2O/MF OR C12H11F5N2/
          MF OR C12H11F6N3/MF OR C12H13F3N2O/MF OR C12H16CLN3/MF OR
          C12H18CLN3O2/MF OR C12H18N2O3/MF OR C12H7F9N2/MF OR C12H8F8N2/M
          F OR C12H9F6N5/MF OR C12H9F7N2/MF OR C13H12F6N2/MF OR C13H12F6N
          2O3S/MF OR C13H12F6N2S/MF OR C13H13CLN2/MF OR C13H13F3N2/MF OR
          C13H13F3N2O2/MF OR C13H13F6N3O2S/MF OR C13H15CLN2/MF OR
          C13H15F3N2O2/MF OR C13H15F3N2O3/MF OR C13H17CLN2O/MF OR
          C13H17F3N2O2/MF OR C13H17F3N2O3/MF OR C13H17F3N2O4/MF OR
          C13H18N2O3/MF OR C13H20N2O3/MF OR C13H8F6N2/MF OR C14H11F9N2O/M
          F OR C14H12F6N2/MF OR C14H13F3N2/MF OR C14H13F6N3O/MF OR
          C14H13F6N3O2/MF OR C14H14F6N2O/MF OR C14H15F3N2/MF OR C14H17CLN
          2/MF OR C14H17F3N2O/MF OR C14H17F3N2O3/MF OR C14H17N3/MF OR
          C14H19CLN2/MF OR C14H19F3N2O2/MF OR C14H20N2O2/MF OR C14H22N2O2
          /MF OR C15H14F6N2/MF OR C15H16F6N2/MF OR C15H17F3N2O2/MF OR
          C15H19N3O2/MF OR C15H21CLN2/MF OR C15H21CLN2O2/MF OR C15H21F3N2
          O2/MF OR C15H21N3O2/MF OR C15H24N2O2/MF OR C16H19F3N2/MF OR
          C16H19F3N2O2/MF OR C16H20F3NO/MF OR C16H21F3N2O/MF OR C16H21F3N
          2O2/MF OR C17H12F9N/MF OR C17H19F6N3O2/MF OR C17H23F3N2/MF OR
          C17H25N3O2/MF OR C18H27F3N4/MF OR C21H31F3N2OSI/MF OR C9H6F6N2O
          2/MF)
L56     359 SEA SPE=ON  ABB=ON  PLU=ON  L55 AND L38

          FILE 'ZCAPLUS' ENTERED AT 10:56:37 ON 12 MAR 2009
L57      68 SEA SPE=ON  ABB=ON  PLU=ON  L56
L58      49 SEA SPE=ON  ABB=ON  PLU=ON  L57 AND P/DT
L59      19 SEA SPE=ON  ABB=ON  PLU=ON  L57 NOT L58
L60      16 SEA SPE=ON  ABB=ON  PLU=ON  L59 AND PY<2004
L61      28 SEA SPE=ON  ABB=ON  PLU=ON  L58 AND PD<20030610
L62      35 SEA SPE=ON  ABB=ON  PLU=ON  L58 AND PRD<20030610
L63      30 SEA SPE=ON  ABB=ON  PLU=ON  L58 AND AD<20030610
L64      51 SEA SPE=ON  ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63)
          D COST
L65      1 SEA SPE=ON  ABB=ON  PLU=ON  L54 AND L1

          FILE 'REGISTRY' ENTERED AT 10:59:42 ON 12 MAR 2009
L66     142 SEA SPE=ON  ABB=ON  PLU=ON  L55 AND L54
L67     366 SEA SPE=ON  ABB=ON  PLU=ON  L56 OR L66

          FILE 'ZCAPLUS' ENTERED AT 11:00:41 ON 12 MAR 2009
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L68	68	SEA	SPE=ON	ABB=ON	PLU=ON	L67
L69	1	SEA	SPE=ON	ABB=ON	PLU=ON	L68 AND L1
L70	51	SEA	SPE=ON	ABB=ON	PLU=ON	L68 AND L64

FILE 'REGISTRY' ENTERED AT 11:02:00 ON 12 MAR 2009

FILE 'ZCAPLUS' ENTERED AT 11:02:04 ON 12 MAR 2009

D STAT QUE L69

D IBIB ABS HITSTR L69 1

FILE 'REGISTRY' ENTERED AT 11:02:42 ON 12 MAR 2009

D STAT QUE L70

FILE 'ZCAPLUS' ENTERED AT 11:02:50 ON 12 MAR 2009

D IBIB ABS HITSTR L70 1-51

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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DICTIONARY FILE UPDATES: 11 MAR 2009 HIGHEST RN 1119363-64-2

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FILE ZCAPLUS

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FILE COVERS 1907 - 12 Mar 2009 VOL 150 ISS 11

FILE LAST UPDATED: 11 Mar 2009 (20090311/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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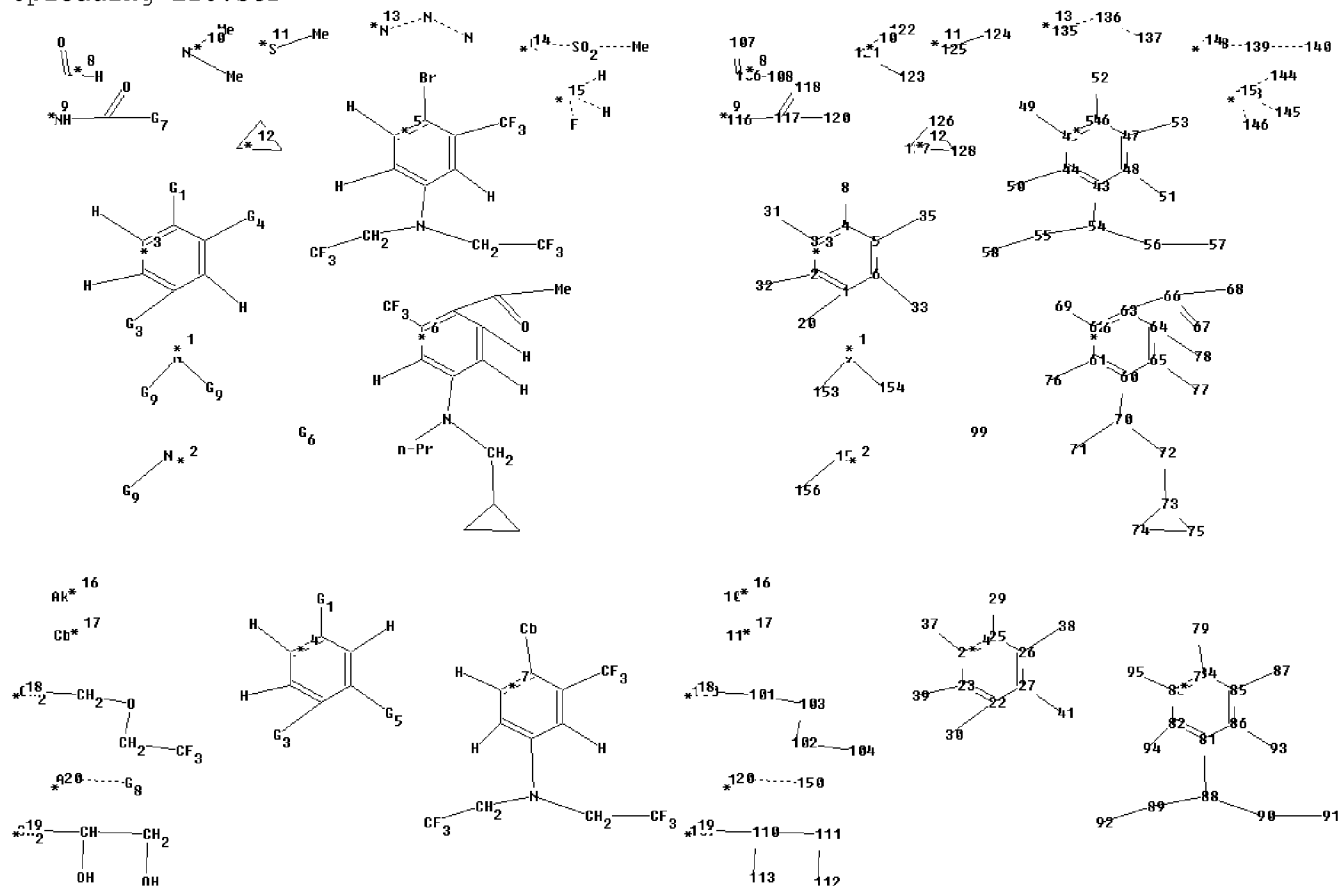
FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Mar 6, 2009 (20090306/UP).

=>

Uploading L26.str



chain nodes :

8 9 10 11 15 20 29 30 31 32 33 35 37 38 39 41 49 50 51 52 53
54 55 56 57 58 66 67 68 69 70 71 72 76 77 78 79 87 88 89 90 91
92 93 94 95
99 100 101 102 103 104 106 107 108 109 110 111 112 113 115 116 117
118 120 121
122 123 124 125 135 136 137 138 139 140 143 144 145 146 150 153 154
156

ring nodes :

1 2 3 4 5 6 22 23 24 25 26 27 43 44 45 46 47 48 60 61 62 63
64 65 73 74 75 81 82 83 84 85 86 126 127 128

chain bonds :

1-20 2-32 3-31 4-8 5-35 6-33 9-153 9-154 15-156 22-30 23-39 24-37 25-29
26-38 27-41 43-54 44-50 45-49 46-52 47-53 48-51 54-55 54-56 55-58 56-57
60-70 61-76
62-69 63-66 64-78 65-77 66-67 66-68 70-71 70-72 72-73 79-84 81-88 82-94
83-95 85-87
86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-108

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106-107 109-110
110-111 110-113 111-112 115-150 116-117 117-118 117-120 121-122 121-123
124-125 135-136
136-137 138-139 139-140 143-144 143-145 143-146
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 73-74 73-75
74-75 81-82
81-86 82-83 83-84 84-85 85-86 126-127 126-128 127-128
exact/norm bonds :
1-20 4-8 5-35 9-153 9-154 15-156 22-30 25-29 27-41 43-54 60-70 66-67
73-74 73-75 74-75 81-88 106-107 110-113 115-150 116-117 117-118 117-120
126-127 126-128
127-128 135-136 136-137 138-139 139-140 143-144 143-145 143-146
exact bonds :
2-32 3-31 6-33 23-39 24-37 26-38 44-50 45-49 46-52 47-53 48-51 54-55
54-56 55-58 56-57 61-76 62-69 63-66 64-78 65-77 66-68 70-71 70-72 72-73
79-84 82-94 83-95
85-87 86-93 88-90 88-89 89-92 90-91 100-101 101-103 102-103 102-104 106-
108 109-110
110-111 111-112 121-122 121-123 124-125
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 43-44 43-
48
44-45 45-46 46-47 47-48 60-61 60-65 61-62 62-63 63-64 64-65 81-82 81-86
82-83 83-84
84-85 85-86
isolated ring systems :
containing 1 : 22 : 43 : 60 : 81 :
```

G1:CN,NO2

G3:[*1],[*2]

G4:CF3,C1,NO2,CH3,OH,CN

G5:CH3,CF3,NO2,C1

G6:[*3],[*4],[*5],[*6],[*7]

G7:CH3,MeO,t-BuO

G8:CF3,OH,MeO,EtO,NH2,[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15]

G9:[*16],[*17],[*18],[*19],[*20]

Hydrogen count :

9:= exact 0 15:= exact 1

Connectivity :

9:3 E exact RC ring/chain 10:1 E exact RC ring/chain 11:1 E exact RC ring/chain
15:2 E exact RC ring/chain 79:1 E exact RC ring/chain 115:2 E exact RC ring/chain
125:2 E exact
RC ring/chain 126:2 E exact RC ring/chain 128:2 E exact RC ring/chain 138:2 E
exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
15:CLASS 20:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 29:CLASS

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30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS 37:CLASS 38:CLASS 39:CLASS 41:CLASS 43:Atom
44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS
54:CLASS 55:CLASS
56:CLASS 57:CLASS 58:CLASS 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom
66:CLASS
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom
75:Atom 76:CLASS 77:CLASS
78:CLASS 79:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:CLASS
88:CLASS
89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 95:CLASS 99:CLASS
100:CLASS 101:CLASS
102:CLASS 103:CLASS 104:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 111:CLASS
112:CLASS 113:CLASS 115:CLASS 116:CLASS 117:CLASS 118:CLASS 120:CLASS
121:CLASS 122:CLASS
123:CLASS 124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 135:CLASS 136:CLASS
137:CLASS
138:CLASS 139:CLASS 140:CLASS 143:CLASS 144:CLASS 145:CLASS 146:CLASS
150:CLASS 153:CLASS
154:CLASS 156:CLASS

Generic attributes :

11:

Saturation : Saturated

79:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 10: Limited

C,C7

Node 11: Limited

C,C6

Node 79: Limited

C,C6

Node 115: Limited

C,C6